ATOM XT Series Manual

Total Sulfur and Total Nitrogen in Liquids, Gases and LPG Laboratory Analyzer

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About This Manual

This is a multipart user's manual that provides information regarding the proper installation, operation and service of ATOM Instrument's XT Series Total Sulfur and/or Total Nitrogen Laboratory Analyzers.

The contents of this document are subject to change without notice. All technical information in this document is for reference purposes only. System configurations and specifications in this document supersede all previous information received by the purchaser.

COSA Xentaur makes no representations that this document is complete, accurate or error-free and assumes no responsibility and will not be liable for any errors, omissions, damage or loss that might result from any use of this document, even if the information in the document is followed properly.

Warranty, compliance, and safety information concerning the XT Series Total Sulfur and/or Total Nitrogen Laboratory Analyzer is provided in the next section.

The benefits, features and configurations of the XT Series are described along with basic theory and operations.

Installation and operation of the XT analyzers and most optional equipment are illustrated in subsequent sections of this manual. Future Information may be supplied in other manuals (i.e., modules manuals) or addenda to this manual.

Maintenance information includes step-by-step procedures along with a complete set of drawings and schematics.

The information contained herein is furnished without warranty of any kind. Users should consider the data in this manual only as a supplement to other information gathered by them and must make independent determinations of the suitability and completeness of the information.

Some of the terms and labels used in the manual are abbreviated intuitively due to space constraints in tables, photos and illustrations. For further explanation, contact ATOM Instrument service.

Also, note that for ease of redaction and reading, all tabs, subtabs, sub-subtabs, etc. will be called tabs and will be designated by their name throughout all of this manual.

Conditions for Proper Use of Instrument

The ATOM XT Series laboratory analyzers are designed to be installed, operated and maintained as specified in this manual. Failure to operate the analyzers as specified may produce erroneous data and possible equipment failure which may void the warranty. Some of the conditions for proper and improper use of the XT laboratory analyzers are provided as follows:

- The XT laboratory analyzers are designed to analyze liquid samples from an autosampler or gas/LPG samples from an External Injection Module (EIM) and display the amount of total sulfur and/or total nitrogen contained in the sample. Operation for any use other than specified may damage the analyzer and/or cause personal injury to the operator. The results obtained for any other use cannot be guaranteed.
- The standard configuration of the XT laboratory analyzers is not intended for use outside of laboratory environments.
- The best accuracy and precision is obtained when the analyzer is located in a temperature controlled laboratory.
- The electrical power source for the analyzer must be capable of delivering 1400 Watts (minimum) of power. The Input power is split into two entries – the furnace side and the electronics side. The total maximum power drawn by furnace side is 1300 Watts and the electronics side is 100 Watts.
- Air and other gases supplied to the analyzer should be filtered and meet specified purity requirements. The recommended purity for all gases is Ultra High Purity (UHP) except when using air for combustion in sulfur-only applications, which should be zero-grade.
- Install the instrument in a place where open fire is not used. Failure to do so has the potential for a fire hazard.
- Install the instrument in a place where there is no possibility of water entering the system as it can potentially be a shock hazard.
- Since flammable gases will be used, install the instrument in a well-ventilated area. Failure to do so has the potential for a fire hazard.
- Releasing gases into an occupied room can also be a severe health risk.
- Ensure that all relevant safety precautions are carefully followed and all gas lines, regulators, gas purifiers, etc. are specified for the intended use.
- **All cautions and warnings in this manual pertaining to the installation, operation and maintenance of the analyzer must be read carefully and observed. Ignoring warning and caution messages can cause equipment damage and possibly lead to personal injury. Operating the instrument incorrectly, or outside its recommended scope will also void any factory warranty.**
- **For any questions or concerns regarding the Analyzer and its use, please contact the COSA XENTAUR office for support.**

Instructions for proper lifting and handling of Analyzer and peripheral modules

The ATOM analyzer and its peripheral modules consist of delicate parts, and at the same time, some of the equipment can be heavy as well as cumbersome to handle. Hence the instrument should be handled with proper care.

- Make sure the Analyzer and its peripheral modules are powered OFF before moving them.
- Verify that all inter-connections between modules have been disconnected before moving any equipment.
- DO NOT move analyzer and/or EIM unless samples and gas bottles have been disconnected from the instruments and the internal tubing has been de-pressurized.
- DO NOT move the analyzer with the Autosampler module still installed on top of the analyzer.
- DO NOT move the Autosampler unless the sample and wash vials, as well as the input module have been disconnected from the unit.
- Move each analyzer module separately.
- Use proper lifting techniques when picking up equipment.
- Wear protective gear such as gloves and steel toed boots to minimize injuries.
- Use additional personnel when handling equipment around tight spaces, especially the analyzer modules that are heavy.
- It is strongly recommended that you use a sturdy cart to safely move analyzer and its modules.

Disposal of Analyzer and peripheral modules

The ATOM analyzer and its peripheral modules are used for analyzing Sulfur and Nitrogen contents in hydrocarbons. These are potentially toxic and harmful as well as pose an environmental hazard. Hence there are certain recommended guidelines that should be followed to dispose of the analyzer and/or its peripheral modules.

- DO NOT dispose Analyzer and/or its peripheral modules in regular trash.
- The syringe must be removed from Autosampler module and disposed of separately as a biohazard before disposing of the entire module.
- Any unused sample, such as liquid in sample vials, should be disposed of before disposing of the instrument itself.
- The Analyzer uses a glass/quartz tube as a combustion chamber. This should be removed from the analyzer and treated as a biohazard and disposed accordingly.
- The external tubing carrying sample to the Analyzer and/or its peripheral modules should not be disposed of into regular trash.
- Refer to EPA and OSHA guidelines for latest information regarding disposing potentially hazardous waste and equipment.
- Contact third party instrument recycling companies for information on offered programs.
- Contact the COSA XENTAUR office for support.

Service

Service Contact Information

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Analyzer models based on application and combustion/carrier gas requirements

MODEL	Sulfur Measurement	Nitrogen Measurement		Uses Zero Air	Uses Oxygen	Uses Argon
XTS-1000	✓			✓		
XTS-1000-O	✓				✓	✓
XT-2000- SA	✓			✓		
XT-2000-S	✓				✓	✓
XT-2000-N		✓			✓	✓
XT-2000-SN	✓	✓			✓	✓

Recommended Consumable and Spare Parts List for Air Units

For models: XTS-1000 and XT-2000-SA

Part Number	Description	Quantity
23305-00001	Syringe, 10uL	2
23304-00001	Septum, 9.5mm, 10 pk	1
23306-00001	Vial w/cap, Screw, 12x32mm, Clear, 100 pk	1
11228-00001	Membrane Dryer	1
60064-00001	Combustion tube	1
10027-00001	Graphite Ferrule, 1/4", 2 pk	1
23251-00001	Tubing, PTFE, 10 ft.	1
23252-00001	Ferrule, set, 1/8" SS, 10 pk	1
60097-10006	Thermocouple, Furnace	1
60001-10001	Excimer Lamp assembly	1
60038-00002	Furnace, 8 in	1

Recommended Consumable and Spare Parts List for Argon/Oxygen Units

For models: XTS-1000-O, XT-2000-S, XT-2000-N and XT-2000-SN

Part Number	Description	Quantity
23305-00002	Syringe, 25uL	2
23304-00001	Septum, 9.5mm, 10 pk	1
23306-00001	Vial w/cap, Screw, 12x32mm, Clear, 100 pk	1
11228-00002	Heated Membrane Dryer (for Sulfur units)	1
11228-00004	Dryer, 2FT (for Nitrogen units)	1
60064-00001	Combustion tube	1
10027-00001	Graphite Ferrule, 1/4", 2 pk	1
23251-00001	Tubing, PTFE, 10 ft.	1
23252-00001	Ferrule, set, 1/8" SS, 10 pk	1
60097-10006	Thermocouple, Furnace	1
60001-10001	Excimer Lamp assembly	1
60038-00002	Furnace, 8 in	1

Section 1 – Principle of Operation, Drawings and Ratings

Section 1.1 – Principle of Operation

The XT Series are laboratory analyzer designed for the measurement of Total Sulfur and/or Total Nitrogen. The schematic below *(Figure 1)* displays the various elements contained in the analysis chain:

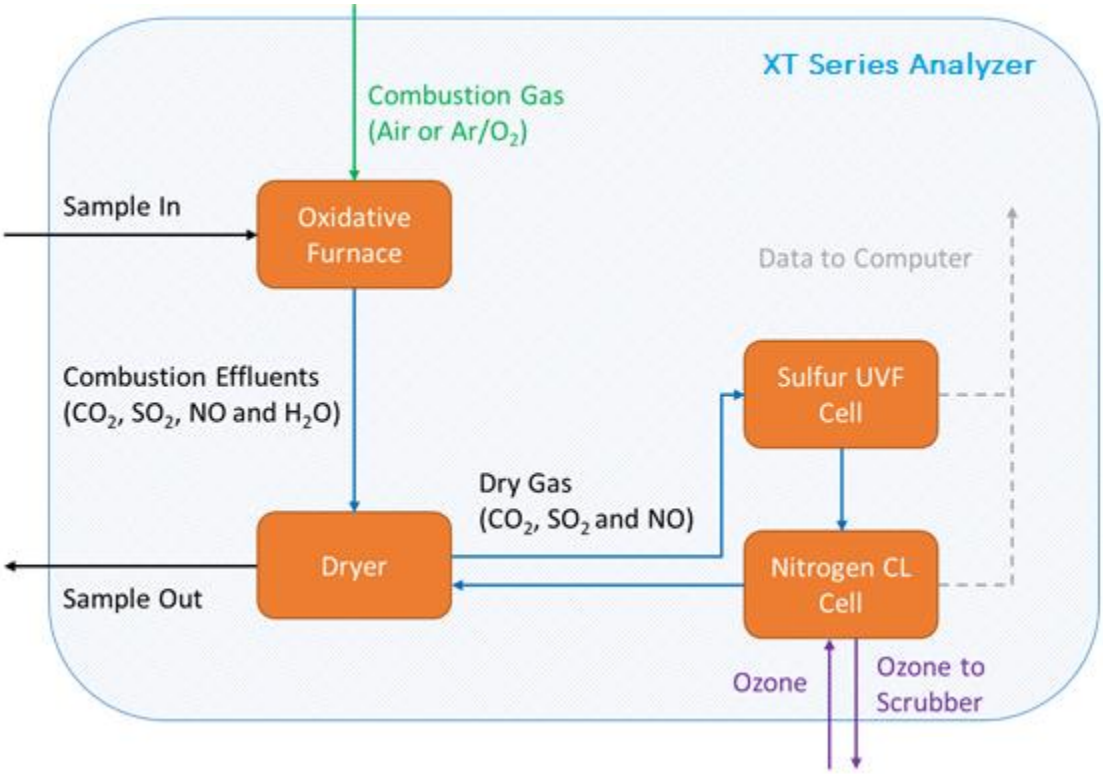


Figure 1 Schematic of Analyzer

Flow Path:
The analysis cycle starts with the injection of the sample into a combustion furnace where hydrocarbon samples are oxidized to CO_2, H_2O, SO_2 and NO. The combustion tube effluent is then directed to flow through a membrane dryer for water removal. The membrane drier outlet is then directed to the Total Sulfur and/or Total Nitrogen detection cells. Section 1.2 details the physiochemistry of both measurements.

Data Collection:
A typical analysis consists of the passage of a sample through all the analyzer parts and the resulting data collected by the computer. Each sample is analyzed as the detector response (in counts) versus time. As the sample goes through the analyzer, various timed events are performed as part of the analysis.

Timed Events:
The analysis begins with the injection of the sample in the furnace and in parallel, the evaluation of the signal baseline noise which is then mathematically removed from sample response. Once the sample has reached the detector, the resulting response is recorded by the computer in the form of a counts peak.

At the end of the analysis, the surface area of the peak is calculated to measure Total Sulfur and/or Total Nitrogen concentration.

Section 1.2 – Principle of Measurement

Section 1.2.1 – Total Sulfur Measurement

The ATOM XT Series utilize patented Excimer UV Fluorescence (EUVF) technology to measure Total Sulfur in a variety of products.

The UV Fluorescence method (UVF) is one of the most simple and practical low-level sulfur analytical techniques that has been widely used and proven over many years of industrial utilization. The UV Fluorescence method involves injection of a sample into a high-temperature oxidation or combustion furnace, which converts all hydrocarbons into water (H_2O) and carbon dioxide (CO_2) byproducts. Total Sulfur content contained in any molecular-bound hydrocarbon species is similarly oxidized at temperatures in excess of 1000°C into sulfur dioxide (SO_2) by the reaction:

$$R\text{-}SH + O_2 \rightarrow SO_2 + CO_2 + H_2O$$

The furnace effluent containing these combustion byproducts is directed into a detection chamber where it is excited by high-energy, short-wavelength emission from a UV excitation source. The UV photons from the excitation source or lamp, transfers energy into the SO_2 molecule and raises its energy level to create an excited singlet state. These excited molecules rapidly decay back to their lower energy ground state releasing the absorbed energy as a secondary emission known as fluorescence.

$$SO_2 + h\upsilon \rightarrow SO_2^* \rightarrow SO_2 + h\upsilon'$$

This low-level fluorescence emission is optically filtered to remove undesired wavelengths of the UV source and background scatter within the detector chamber. Detection of the filtered fluorescence emission is usually accomplished with a Photomultiplier Tube (PMT), Channel-Plate Multiplier (CPM) or other high gain, light-sensitive detector.

Section 1.2.2 – Total Nitrogen Measurement

The XT Series may also be configured for the measurement of Total Nitrogen utilizing the nitrogen chemiluminescence method for a variety of applications and products.

Nitrogen chemiluminescence is the most widely used analytical technique for low-level measurement of total nitrogen and has proven over many years of industrial utilization.

This chemiluminescence method starts with the injection of a sample into a high-temperature oxidation or combustion furnace. Although some applications may include the analysis of non-hydrocarbon-based products, hydrocarbons are typically converted into water (H_2O) and carbon dioxide (CO_2) byproducts. Total Nitrogen content of molecularly-bound compounds is similarly oxidized at temperatures in excess of 1000°C to nitric oxide (NO) by the reaction:

$$R\text{-}NH + O_2 \rightarrow \cdot NO + CO_2 + H_2O$$

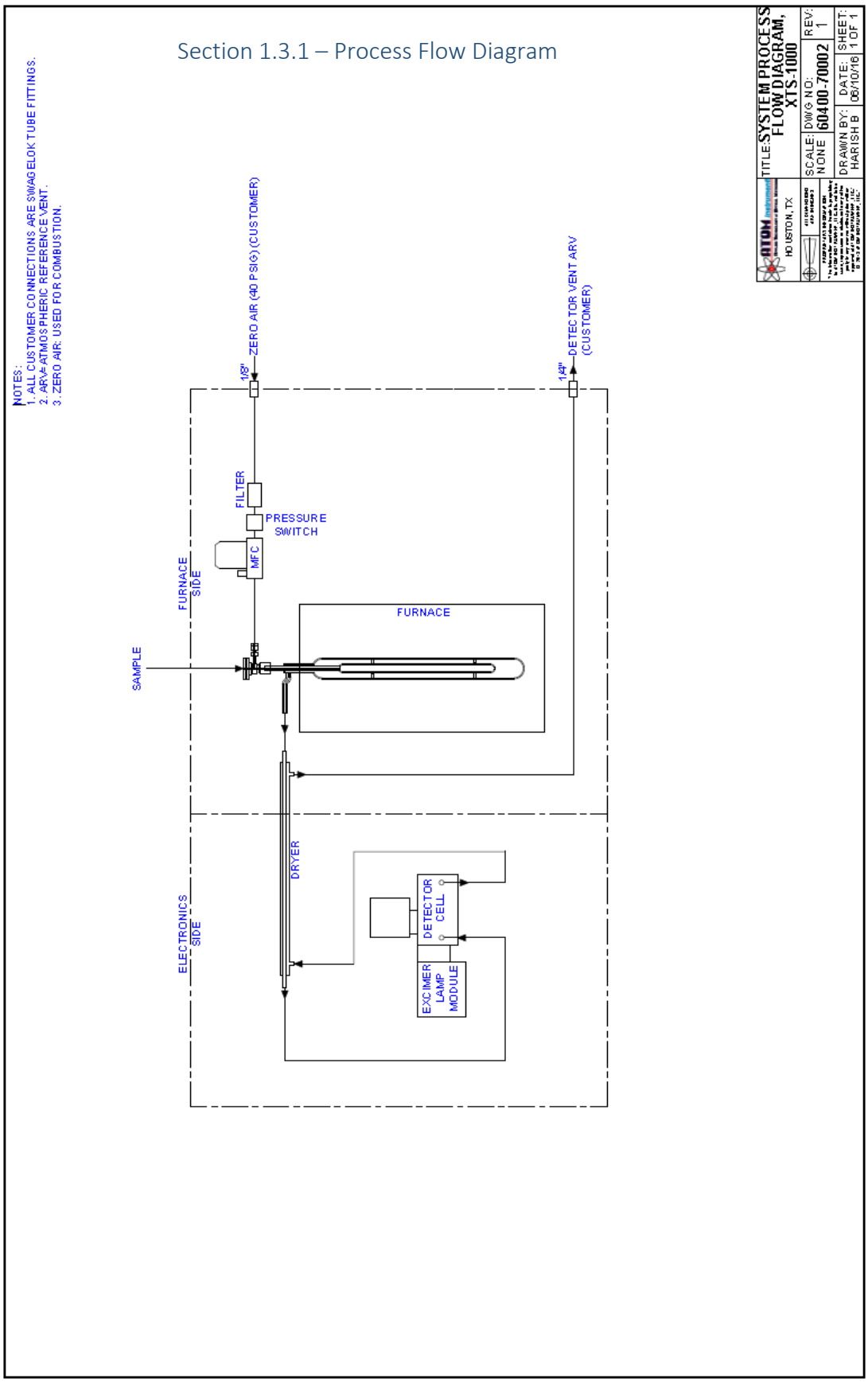
The furnace effluent containing these combustion byproducts is directed into the detection chamber where nitric oxide (·NO) reacts with ozone to form Nitrogen Dioxide (NO_2):

$$\cdot NO + O_3 \rightarrow NO_2 + O_2 + h\upsilon$$

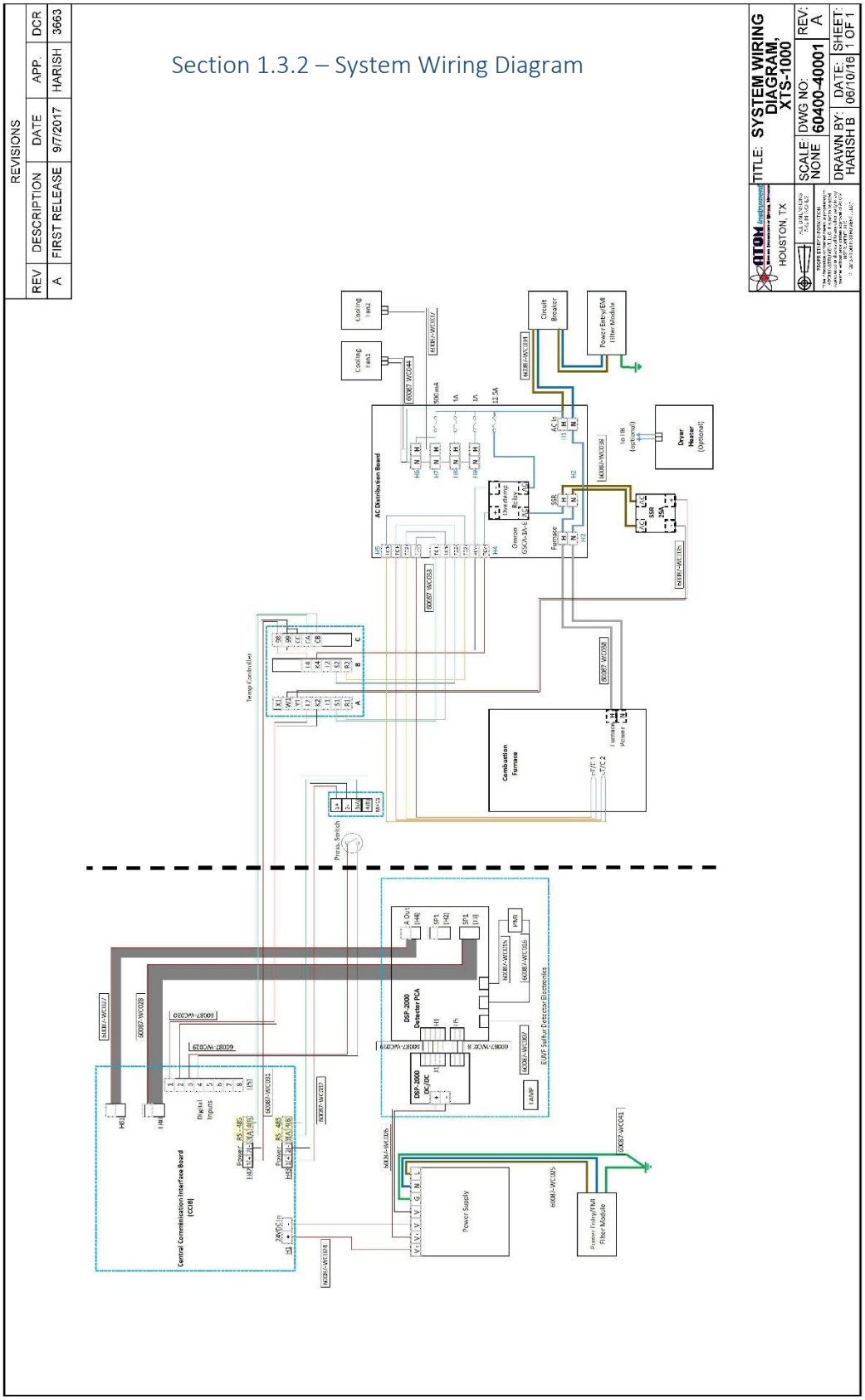
The interaction of Ozone (O_3) and Nitric Oxide (·NO) generates photons causing an emission of light known as chemiluminescence which is proportional to the nitric oxide concentration. Detection of the emission is usually accomplished with a Photomultiplier Tube (PMT), Channel-Plate Multiplier (CPM) or other high gain, light-sensitive detector.

Section 1.3 – XTS-1000 Drawings

Section 1.3.1 – Process Flow Diagram



Section 1.3.2 – System Wiring Diagram



Section 1.4 – XT-2000 Drawings

Section 1.5 – Electrical Ratings

Section 1.5.1 – XT Series Analyzer

Model	XTS-1000	XT-2000 – 110 VAC	XT-2000 – 220 VAC
Voltage Rating	100-120 VAC	100-120 VAC	210-230 VAC
Current Rating	12 A	13 A	8 A
Max Power Rating	1,440 W	1,560 W	1,840 W

Fuses (110 VAC system): Use 5 X 20 mm fuses with designated ratings only

Amperage	Voltage	Size	Description	Part Number
500 mA	250V	5x20mm	Fan Fuse	11420-00050
1 A	250V	5x20mm	Auxiliary Power	11420-00100
1 A	250V	5x20mm	Heated Dryer Fuse	11420-00100
12.5 A	250V	5x20mm	Furnace Fuse	11420-01250

Fuses (230 VAC system): Use 5 X 20 mm fuses with designated ratings only

Amperage	Voltage	Size	Description	Part Number
500 mA	250V	5x20mm	Fan Fuse	11420-00050
500 mA	250V	5x20mm	Auxiliary Power	11420-00050
500 mA	250V	5x20mm	Heated Dryer Fuse	11420-00050
8 A	250V	5x20mm	Furnace Fuse	11420-00800

Breaker:

- 15A, 275V

Section 1.5.2 – LAS-1000 Autosampler

Voltage Rating	**100-240 VAC**
Current Rating	3 A
Max Power Rating	720 W

Section 1.5.3 – EIM-1000 Gas and LPG External Injection Module

Voltage Rating	**100-230 VAC**
Current Rating	2 A
Max Power Rating	460 W

Section 1.6 – Environmental Operating Condition

Temperature Range: 10°C to 40°C (50°F to 104°F)

Relative Humidity Range: 0% to 90%

Altitude: Up to 2,000 m (6,500 ft)

Section 2 – XT Series Software and Modules Overview

This section of the manual is intended to present an overview of the XT Series programs and modules providing users a fundamental understanding of their interaction.

Section 2.1 – Introduction to Individual XT Series Components

There are three programs (Detector, Scanner and LUI) incorporated into the XT Laboratory Analyzers which have distinct functions but work together to provide complete control and user interface of the XT instruments. A SQL database is used to store the analyzer data: analyzer settings, calibrations and the various analyses results. In addition to the three programs and the SQL database, separate injection modules (Autosampler Robot and/or External Injection Module) make up a complete XT Laboratory Analyzer.

XT Series Software Components	Location
ATOM Detector Software	On Analyzer
ATOM Scanner Service	On Computer
ATOM LUI Software	On Computer
SQL Database	On Computer
XT Series Additional Hardware	
Autosampler Robot	
External Injection Module	

Figure 2 below shows how these individual elements interact with each other, and their methods of communication.

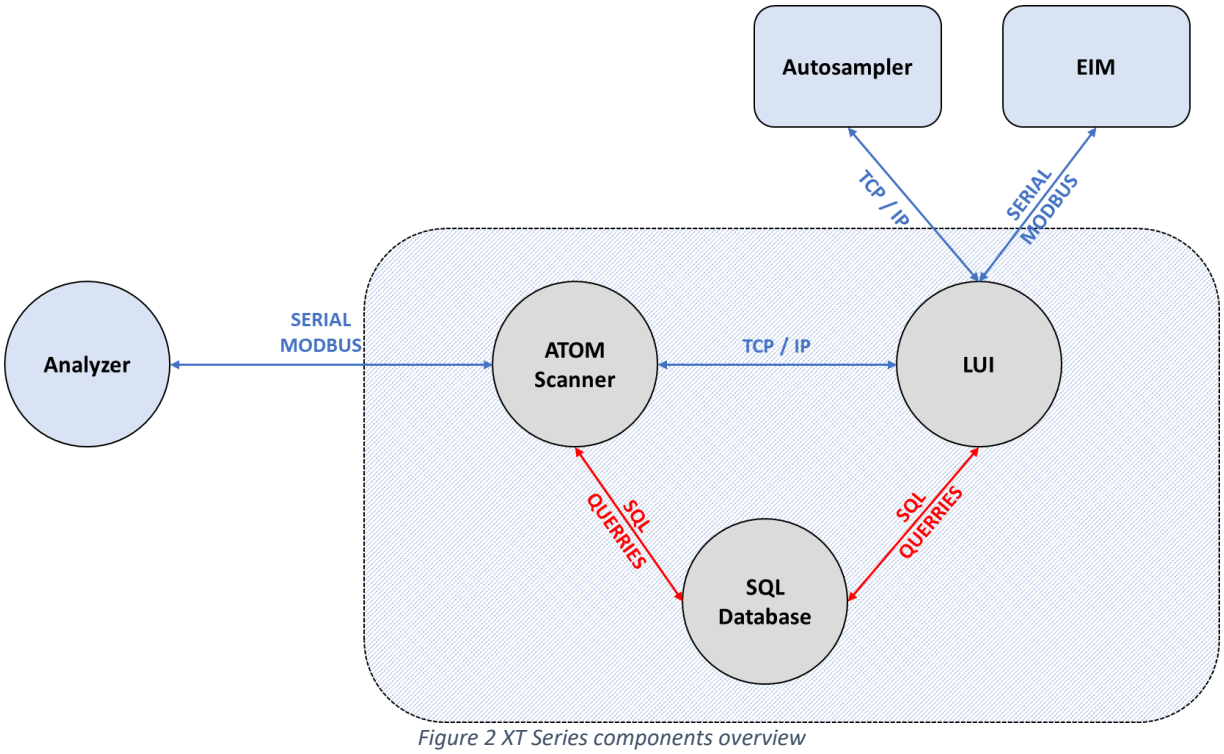


Figure 2 XT Series components overview

Section 2.2 – XT Series Components Functions

1. The ***ATOM Detector*** module firmware is an embedded program internal to the Detector Signal Processor (DSP) circuit board. The software continually reads the output of the PMT and converts detector response into corresponding digital value which, throughout the scope of ATOM documents, is referred to as Detector Count. The detector counts are plotted and represent the associated peak-shape whose underlying area are integrated corresponding to Total Sulfur or Total Nitrogen concentration in the sample.

2. The ***ATOM Scanner Service*** operates in the background as a Windows Service and coordinates communications of all devices between the analyzer and the computer. It controls all aspects of instrument operations with the exception of the Autosampler. The program is a continuous loop that scans all CCIB (*Central Communication Interface Board*) peripherals including Detector board, Mass Flow Controllers (MFC), Temperature Controllers (TC) and external modules. When changes to device readings, status or settings are detected, the scanner updates the SQL database with the current information, and notifies the LUI of the change.

3. The ***ATOM LUI*** (Laboratory User Interface) is a user-friendly graphical interface between the analyzer and users. The LUI allows complete control over the analyzer to create user-defined methods, perform calibration and run analyses. The LUI also communicates user-defined settings to the ATOM Scanner and vice versa. This manual will cover the interaction with the LUI in order to operate the XT analyzers.

4. The ***SQL Database*** is the main communication hub for data between the LUI and the Scanner. It stores all the instrument settings, calibrations and sample analyses data completed to date. Analytical data is preserved and continues to accumulate unless users physically delete the unwanted data.

5. The ***Autosampler*** is the robotic sampling tool used to inject liquid samples in the analyzer. All autosampler parameters are defined and configured within the corresponding method tab in the LUI.

6. The ***External Injection Module (EIM)*** is used to inject LPGs and gases in the analyzer. The EIM is controlled by the ATOM software.

Section 2.3 – Typical Analysis Sequence

This section describes the chain of events occurring during an analysis (Calibration and Sample) and the normal behavior expected from an ATOM XT Series Analyzer

Section 2.3.1 – Autosampler

When using an autosampler, the software will first load the autosampler analysis parameters to the autosampler (Number of Samples, Samples Position, Syringe and Samples Washing instructions, etc…). Once those parameters are loaded, the autosampler will proceed with the first sample by washing the syringe, loading the sample and injecting the sample into the analyzer.

Once the sample is injected into the analyzer, the autosampler will start prepping for the next sample (whether it is another run of the same sample or another sample). While the analyzer is getting ready for the next analysis, the sample is going through the various components of the analyzer (as described in the previous sections) to perform the analysis and generate a Sulfur and/or Nitrogen peak that can be associated with a specific Sulfur/Nitrogen content in the case of a calibration or compared to a calibration in the case of a sample.

Once the sample is analyzed, the autosampler injects the next sample and the cycle repeats until all the samples in the sample set are analyzed. As each sample/standard is analyzed, the information is displayed on the computer for the user.

Note: When using an autosampler, users may load all their samples in the autosampler and leave the analyzer system to perform the analysis of all the samples without the need for external intervention.

Section 2.3.2 – External Injection Module (EIM)

When using an EIM, the overall behavior of the system is similar to that of an autosampler. The most notable difference pertains to sample switching. When using an EIM, a user must manually load each sample between analysis.

The EIM comes in various configuration. On the Liquid/LPG side, the EIM may be manufactured using a high pressure sight glass (1,000 psi / 70 bar) or a flowmeter (500 psi / 35 bar). On the gas side, the valve may be used for 2 different functions. In the first case, as a Gas valve which allows user to analyze gases or as a sample shut off for the liquids/LPG to prevent disposal of sample/standard once the analysis is finished. The table below shows the possible combinations of EIM:

Model	Liquid Side		Gas Side	
	Sightglass	Flowmeter	Gas Valve	Sample Shut Off
EIM-1000-L	X			
EIM-1000-LF		X		
EIM-1000-LSO	X			X
EIM-1000-LFSO		X		X
EIM-1000-G			X	
EIM-1000-GL	X		X	
EIM-1000-GLF		X	X	

Section 2.3.2.1 – Gas Samples

When using a Gas EIM without a sample shutoff, the user must first connect the gas sample to the gas inlet of the EIM. The gas flowmeter allows setting the desired flowrate for the analysis. ATOM recommends setting the flow high enough to have sufficient product circulation through the flow path (Total flowpath volume below 5 cc) but not too high as to not waste sample.

Once the flow is properly adjusted, the software will automatically control the EIM and collect data from the detectors to generate a sample peak and compare to stored calibration in the case of a standard or a specific concentration in the case of a standard.

Once all runs within a samples have been analyzed, the software will prompt the user to load the next sample is other samples remain or finish the sample set if the last run has been performed.

Section 2.3.2.2 – Liquid Samples Without Sample Shut Off (SSO)

When using an EIM without a sample shutoff, the sample will flow freely through the entire flowpath of the EIM once the sample is loaded. Once the sample start flowing through the EIM, users must wait until no more bubbles appear through the sightglass/flowmeter. When using a flowmeter, users may adjust the flow rate to reduce sample usage. ATOM suggests a sample flowrate between 1 and 2 cc/min to ensure proper sample renewal and prevent excessive sample wasting..

If bubbles do not go away, pressure sample might be too low in which case, the sample must be pressurized either by using the sample pressurizing pad feature or by disconnecting the sample and pressurizing it using another means.

Once the flow is properly adjusted, the software will automatically control the EIM and collect data from the detectors to generate a sample peak and compare to stored calibration in the case of a standard or a specific concentration in the case of a standard.

Once all runs within a samples have been analyzed, the software will prompt the user to load the next sample from the sample set. If there are no samples remaining in the sample set, the software will consider the analysis finished.

Section 2.3.2.3 – Liquid Samples With Sample Shut Off (SSO)

When using an EIM with a sample shutoff, the sample will not flow through the flowpath of the EIM until the Sample Shut Off (SSO) is deactivated. Once the sample is loaded, only the path up to the SSO will contain sample.

Once the user initiates the analysis process, the software will deactivate the SSO and allow time to adjust sample flowrate through the EIM to ensure no bubbles are present in the flow path. When using a flowmeter, users may adjust the flow rate to reduce sample usage. ATOM suggests a sample flowrate between 1 and 2 cc/min to ensure proper sample renewal and prevent excessive sample wasting.

If bubbles do not go away, pressure sample might be too low in which case, the sample must be pressurized either by using the sample pressurizing pad feature or by disconnecting the sample and pressurizing it using another means.

Once the flow is properly adjusted, the software will automatically control the EIM and collect data from the detectors to generate a sample peak and compare to stored calibration in the case of a standard or a specific concentration in the case of a standard.

Once all runs within a samples have been analyzed, the software will activate the SSO and prompt the user to load the next sample if other samples remain. If there are no samples remaining in the sample set, the software will consider the analysis finished.

Section 3 – System Setup

The XT Series computer and analyzer software package will arrive pre-installed and ready to use at customer facility.

Please note: Before re-installing any part of the XT software package, please contact ATOM Instrument to verify need of re-installing. To re-install ATOM software package , please uninstall the ATOM redistributables first and the ATOM LUI before proceeding to re-installs on the computer. The installation is done separately for the ATOM Redistributables and the ATOM LUI. The ATOM Scanner is included in the installation of the ATOM LUI Software

Section 3.1 – Installing ATOM Redistributables

When installing software on an ATOM system, always start the installation procedure with the ATOM Redistributables. The ATOM Scanner program is installed via a redistributable file provided by ATOM Instrument.

Double-click on the ATOM Redistributable file to open the installation Wizard *(Figure 3)*.

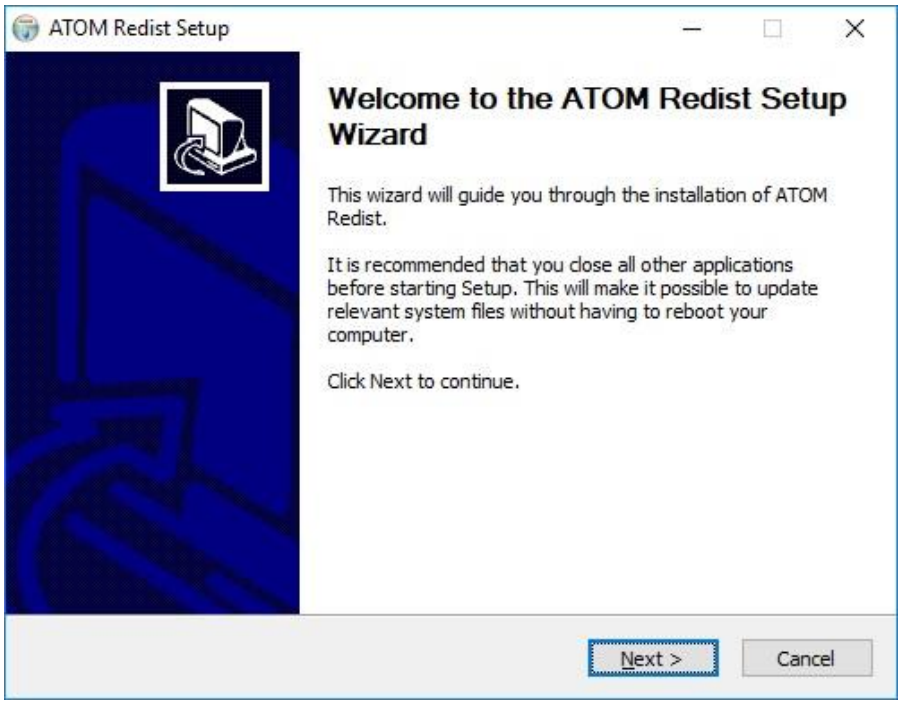


Figure 3 ATOM Redistributable Wizard Installer Screen

Click Next. On the following window select all the components for installation *(Figure 4)* and click Install.

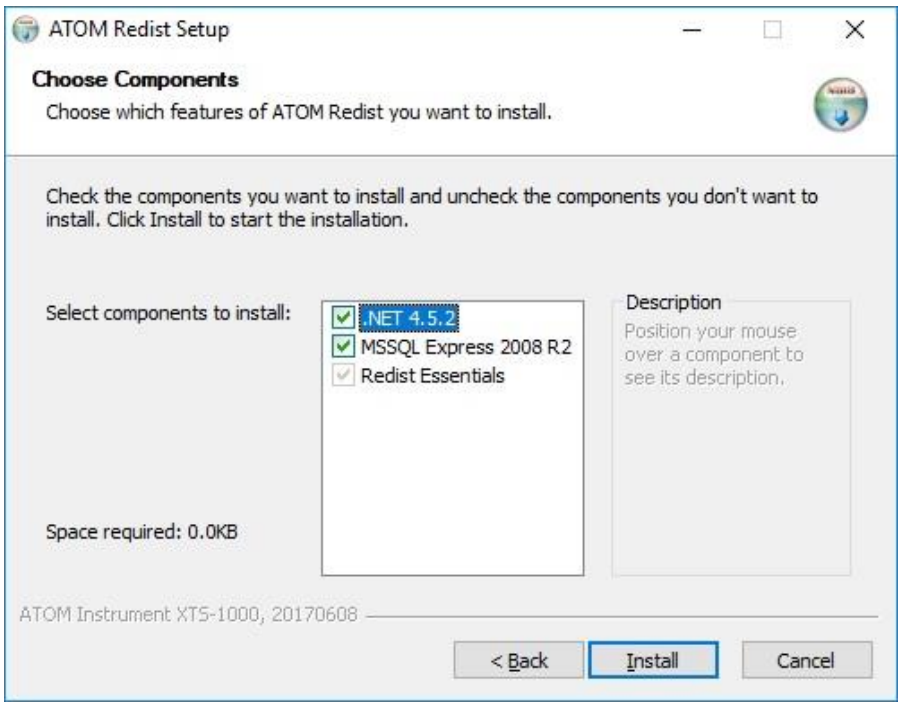


Figure 4 ATOM Redistributable Install Components Choice

Installation takes a few minutes. Once installation is complete *(Figure 5)*, close the Installer and install the LUI.

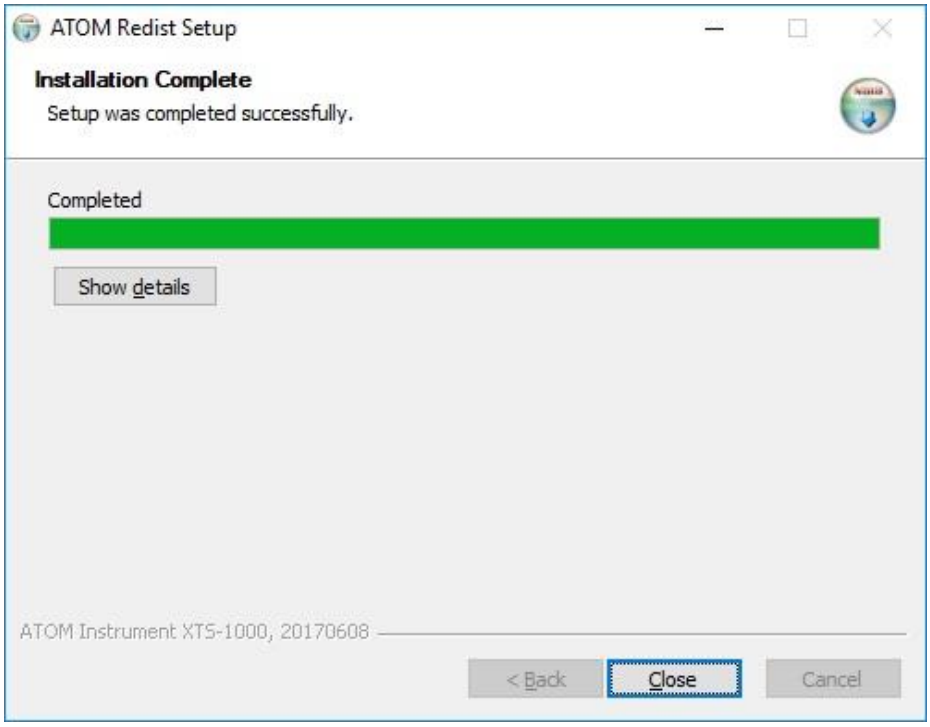


Figure 5 ATOM Redistributable Installation Completion

Section 3.2 – Installing ATOM LUI Software

After successfully completing the installation of the ATOM redistributables, continue with the LUI installation. Please contact ATOM Instrument for the latest version of the LUI software before install.

Double-click on the ATOM LUI Install file to open the installation Wizard *(Figure 6)*.

Figure 6 ATOM LUI Installation Wizard

Click the Next button to proceed with the installation.

On the following window select all the components for installation *(Figure 7)* and click Next.

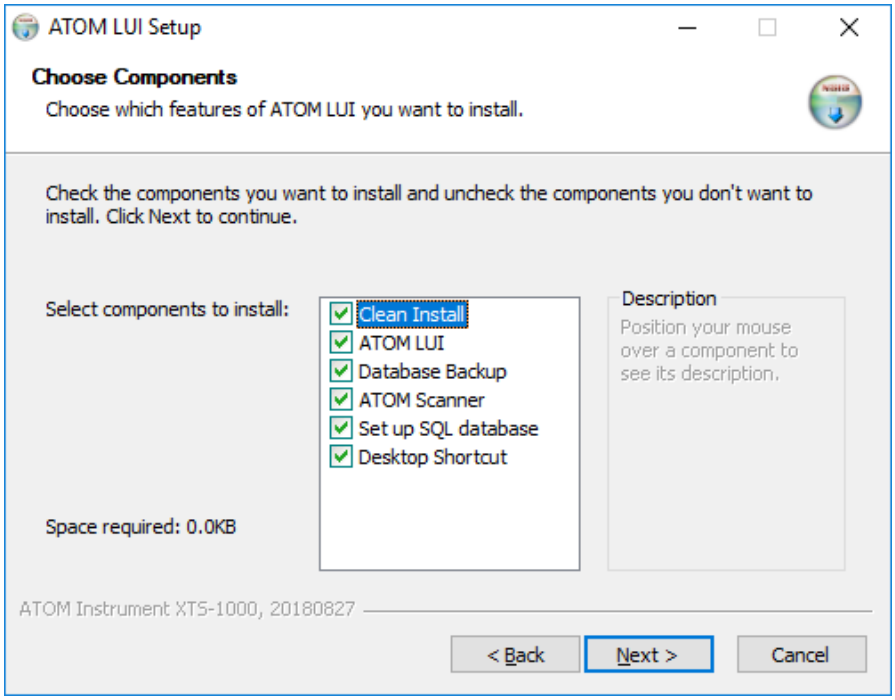


Figure 7 ATOM LUI Install Components Choice

The following window (Figure 8) allows the user to configure the software to match analyzer components and ensure proper communication between the software and the analyzer.

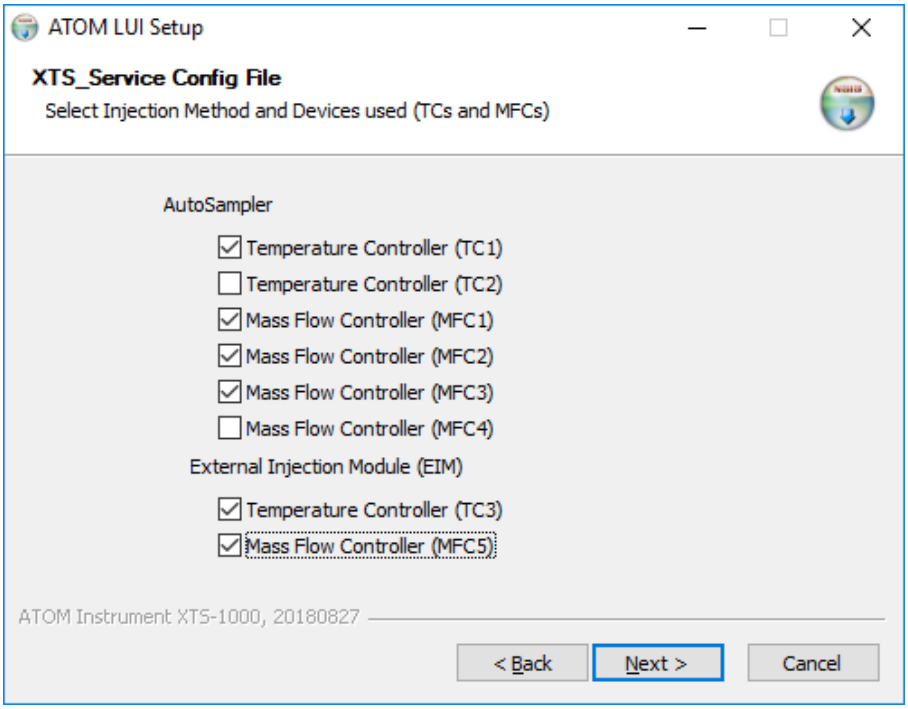


Figure 8 ATOM LUI Components Selection

The table below summarizes the various components options and choices depending on the type of analyzer/EIM. *Note: If the installation does not include and EIM, leave checkboxes TC3 and MFC5 blank.*

XT Series Analyzer						
Oxidizer Type	Air Only		Argon/Oxygen Mixture			
Detector Type	Sulfur		Sulfur		Nitrogen	Sulfur - Nitrogen
Model Type	XTS-1000	XT-2000-SA	XTS-1000-O	XT-2000-S	XT-2000-N	XT-2000-SN
Temperature Controllers						
TC 1	X	X	X	X	X	X
TC 2	Not In Use					
Mass Flow Controllers						
MFC1	X	X	X	X	X	X
MFC2			X	X	X	X
MFC3					X	X
MFC4	Not In Use					

EIM-1000 External Injection Module			
EIM Type	LPG Only	Gas Only	LPG and Gas
Temperature Controller			
TC3		X	X
Mass Flow Controller			
MFC5	X	X	X

Once the appropriate checkboxes are selected click the Next button. The following window (Figure 9) confirms user selection. If the system is properly configured, click next to proceed with the installation. If a component is missing, click back to return to the previous screen an reselect the appropriate components.

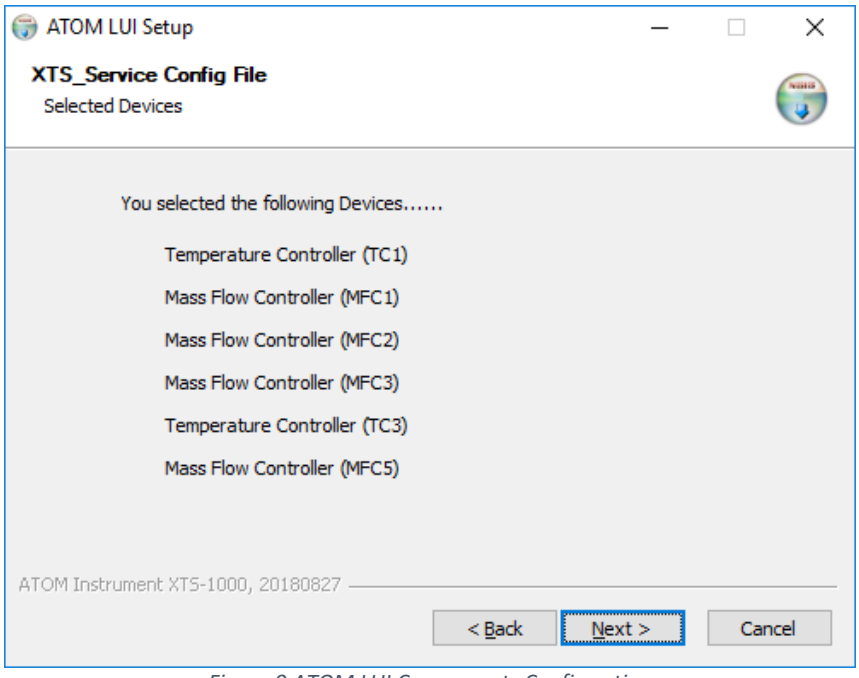


Figure 9 ATOM LUI Components Confirmation

The following window (Figure 10) allows the user to assign to choose the IP address for the autosampler. By default, the autosampler is assigned the IP address 192.168.1.1 in the LUI. If a different address is entered by the user, it must match the address set in the autosampler. To set the address of the autosampler, refer to Section 6.5.1 – Autosampler Network Setup. Once the address has been entered, click "Install" to proceed with the installation.

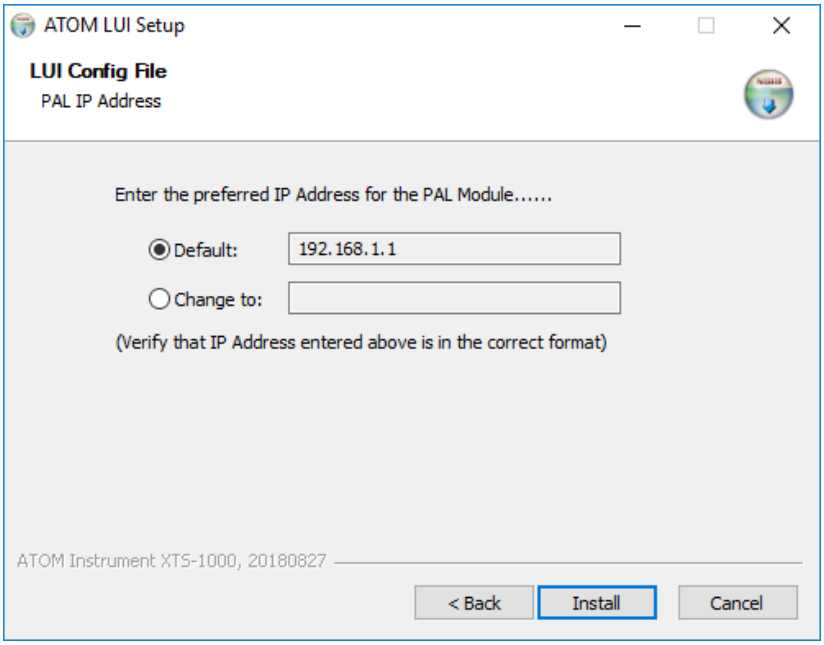


Figure 10 ATOM LUI Autosampler IP Settings

Installation takes a few minutes. Once installation is complete *(Figure 11)*, close the Installer.

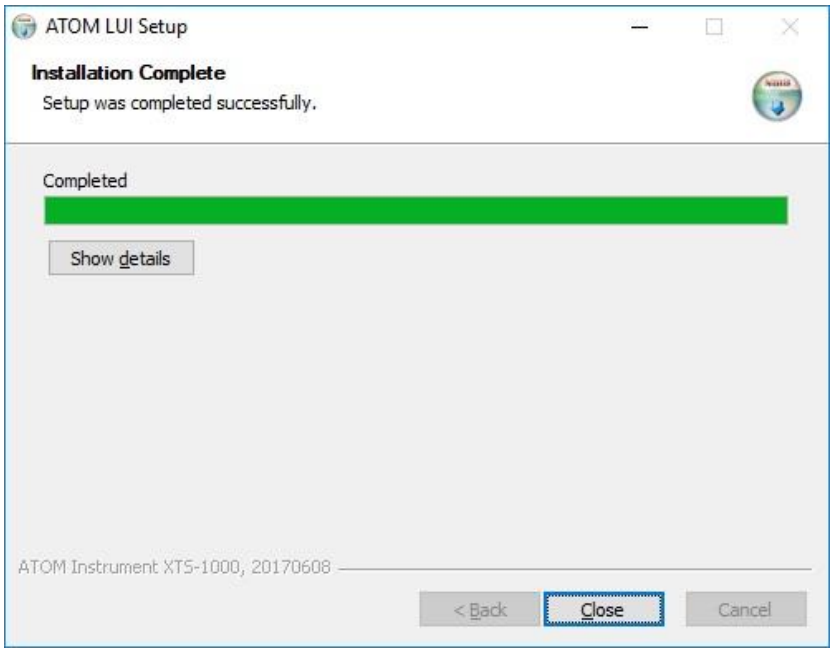


Figure 11 ATOM LUI Install Complete

Section 3.3 – Uninstalling ATOM Scanner Software

To completely remove the ATOM software present on the XT computer, start with the ATOM Redistributable uninstallation before removing the ATOM LUI software.

To remove the ATOM Redistributable, locate the installation folder “ATOM” on the computer. By default, the LUI and Redistributable are installed in the directory: “C:\ATOM”.

In the ATOM folder, double-click on the “uninstallRedist” file to start uninstalling the Redistributables.

When prompted to remove the ATOM Redistributables, click Yes *(Figure 12)*

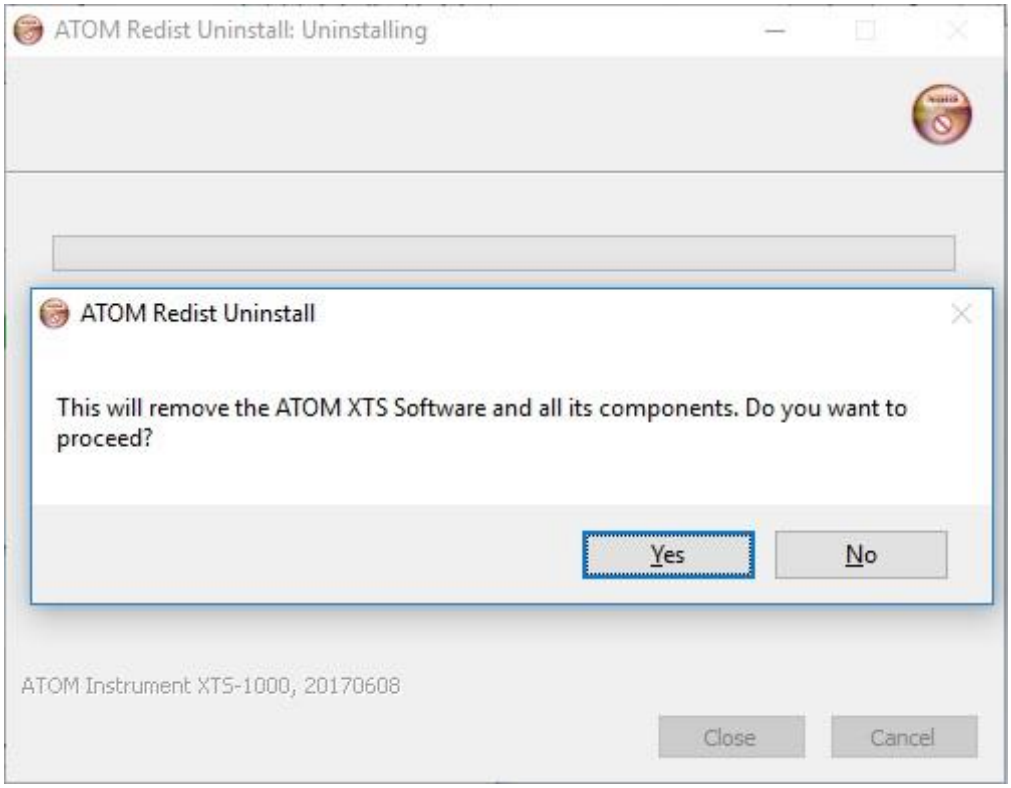


Figure 12 ATOM Scanner Uninstall Wizard

Upon completion, click Close to exit the uninstall Wizard *(Figure 13).*

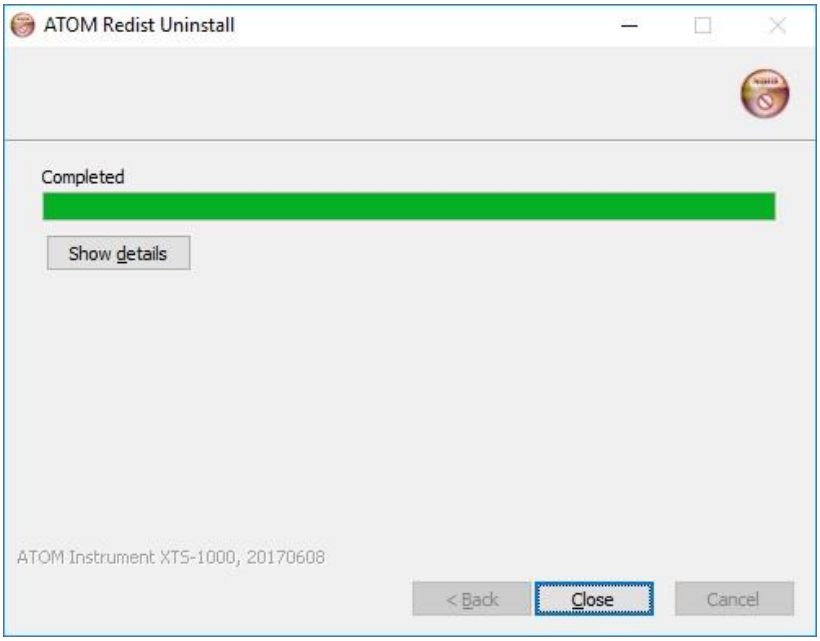


Figure 13 ATOM Scanner Uninstall Complete

Once the ATOM Redistributables are uninstalled, the ATOM LUI may be uninstalled.

Section 3. 4 – Uninstalling ATOM LUI Software

To uninstall the ATOM LUI software located on the ATOM XT computer, locate the "ATOM" folder located by default at: "C:\ATOM".

Double click the "uninstallLUI" file to start the uninstallation process *(Figure 14).*

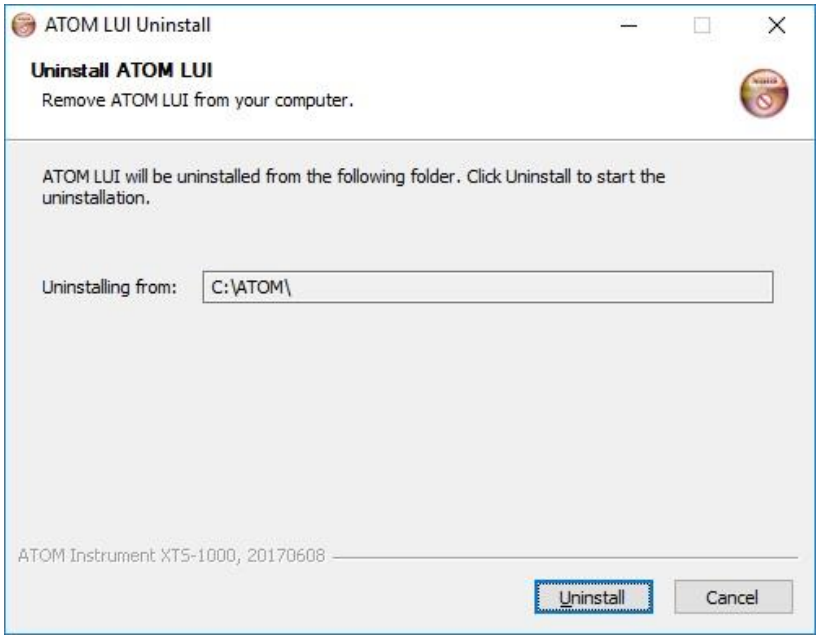


Figure 14 ATOM LUI Uninstall Wizard

Press Uninstall to start removing the ATOM LUI software *(Figure 14)*. Confirm uninstallation in the popup window.

Upon completion of the uninstall click Close to exit the uninstall *(Figure 15).*

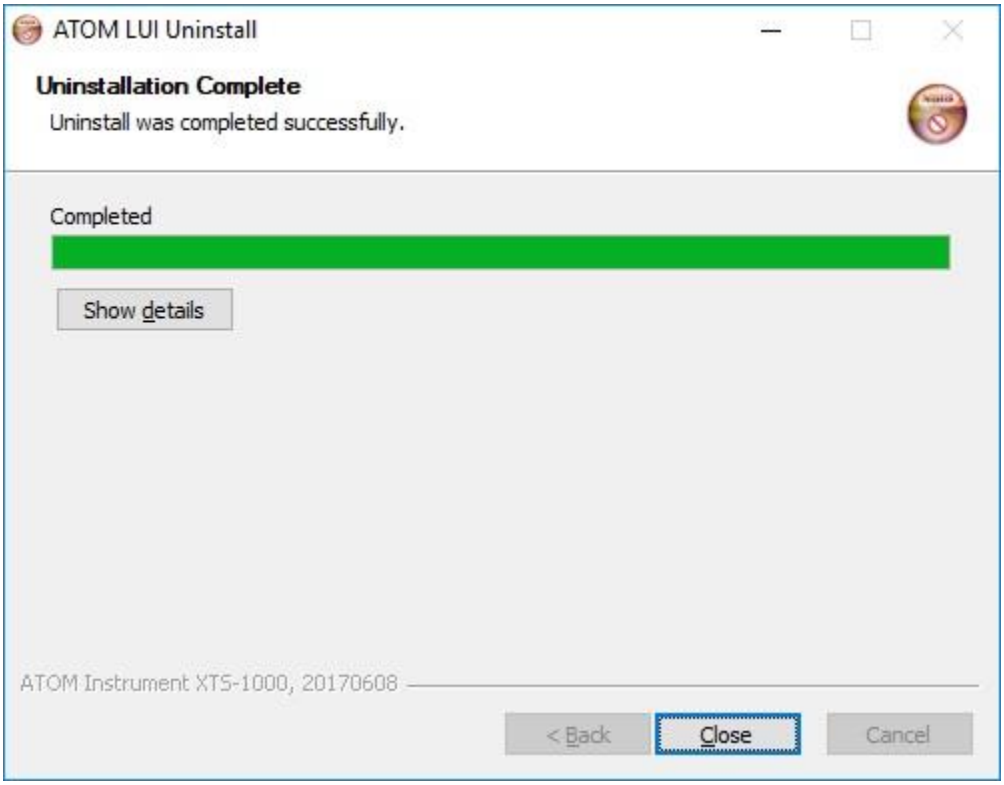


Figure 15 ATOM LUI Uninstall Complete

Section 4 – Quick Start Guide

This section gives a quick overview of software operations regarding: method creation and activation, calibrating and running samples. For detailed information about software operation, please consult Section 5 – Software Operations.

Section 4.1 – Creating a Method

- Select the "Method" tab (*Figure 16*)
- Click the "New" button and select method type

Section 4.2 – Activating a Method

- Select the "Method" tab (*Figure 16*)
- Select the method to activate from the "Method Selection" pane on the left
- Click "Activate" from the buttons below the method name

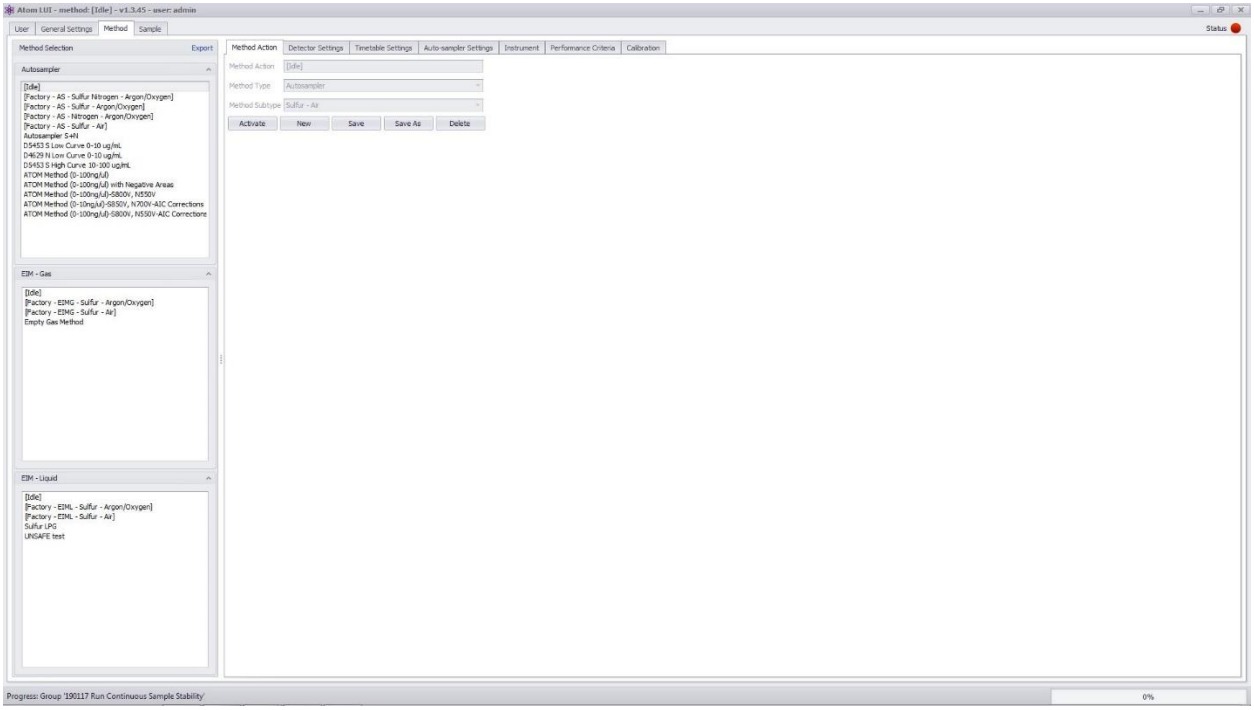


Figure 16 Method Tab

Section 4.3 – Running a Calibration

- Select the “Method” tab at the top of the window
- Activate the method to calibrate *(See Section 4.2 – Activating a Method)*
- Select the “Calibration” tab (*Figure 17*)
- Under the “Calibration Settings” section on the bottom-right:
  - Enter the number of samples (standards) and runs per sample that will be used in the calibration.
  - Set the concentration unit (ng/µl or ppm/wt) and, if ppm/wt, enter the density of standards
  - Fill in the name, tray position, vial position, and concentration information in the table for each standard as they are organized on the autosampler tray.
  - Ensure that each standard is in the correct vial and tray position on the autosampler
- Click the “Run” button at the bottom-right of the screen

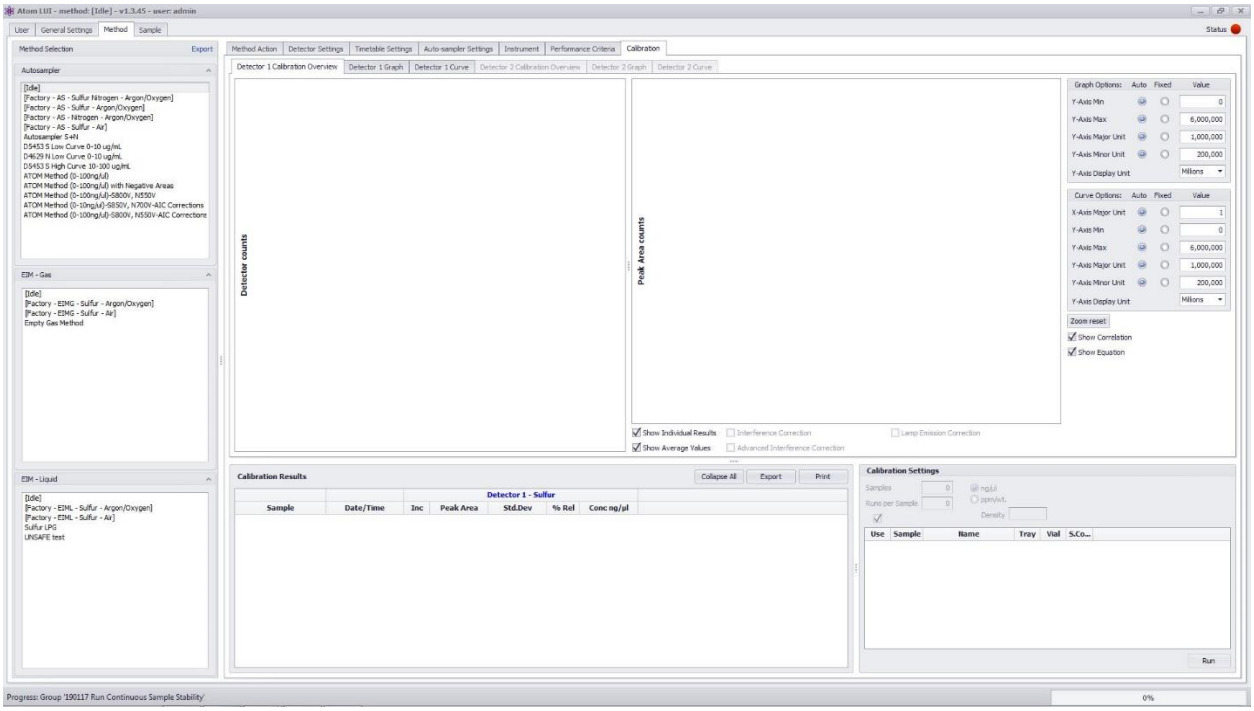


Figure 17 Calibration Tab

Section 4.4 – Running Samples

- Select the “Sample” tab (*Figure 18*)
- Select the group samples will be part of
  - If no group exists, click the “+ Group” button at the top left, and when prompted, name the newly created group
- If the desired samples are not already present in the “Sample Settings” box
  - Press the “+ Sample” button, which will open a new window to enter sample settings
  - Enter the number of samples
  - For any of the input boxes marked with an asterisk (*), any information entered in that box will be cloned across all added samples. If the values are not shared between all samples, leave the entry box blank. When all desired information has been entered, click “OK”. The new samples will be added with blank spaces for incomplete information
- If any changes or additions need to be made to the samples present in Sample Settings, select and enter the necessary values in the corresponding input boxes
- Uncheck the samples from the “Sample Settings” box to deselect the unwanted samples
- Press “Run” at the bottom right of the screen

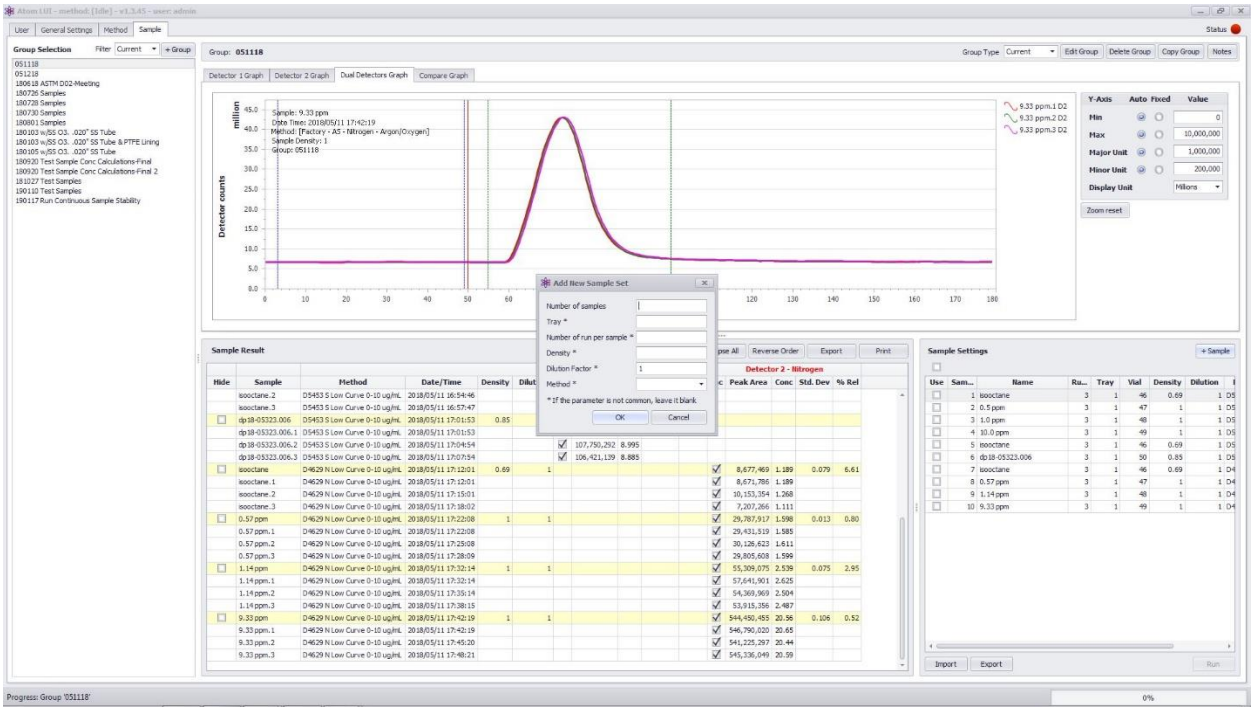


Figure 18 Sample Tab

Section 5 – Software Operations

This section will detail the various screens and tabs contained in the LUI and explain how the software may be operated to run sample analysis and calibrations.

Section 5.1 – Start-Up

When powering up the computer, the scanner software automatically starts-up as a background service. To start the LUI double click on the icon below (*Figure 19*) located on the desktop:

Figure 19 LUI Icon

Section 5.2 – Top Bar and Status Button

The Top Bar of the ATOM LUI software *(Figure 20)* displays the following information: activated method (See Section 5.6.1 – Method Action Tab for more information), software version and current user level (See Section 5.4 – User Tab for more information).

Figure 20 Status Bar and Status Button

To the right hand, the “Underscore” icon minimizes the LUI to the Windows Taskbar, the “Double Window” icon reduces/maximizes the size of the LUI window and the “X” icon closes the LUI.

The radio button status indicator on the right hand side is present on all tabs and windows of the LUI. The radio button uses a 3-color code to indicate operating status: Interrupt, Warning and All Clear.

Section 5.3 – Bottom Status Bar and Progress Bar

The ATOM LUI software features a second Status Bar along with a Progress Bar at the bottom of the screen *(Figure 21)*.

Figure 21 Bottom Status Bar and Progress Bar

The bottom status bar displays information related to ongoing samples and calibration runs and information about operations performed by the software such as exporting and printing. The Bottom Status Bar also features information about aborts and stopped runs.

The Progress Bar on the bottom right indicates the current progress of a calibration or sample run series.

Section 5.4 – User Tab

The user tab is used to administrate user access rights and privileges.

Section 5.4.1 – Overview

The User Tab is used to log in the LUI and administrate user access. The LUI will automatically start up on the User Tab and request a login and password (*Figure 22)*. There are four levels of user: Administrator (Admin), Technician (Tech), Operator (Operator) and Viewer (When not logged in), with the following administrative rights:

	Admin	Tech	Operator	View
View any LUI tab	X	X	X	X
Run samples	X	X	X	
Modify and create methods	X	X		
Modify user privileges	X			

An administrator is the only user allowed to modify all user privileges (*Figure 23)*. Other logged in users may change their password on the User tab *(Figure 24)*.

Note: Passwords and usernames are not case sensitive

Figure 22 User Tab – Login Screen

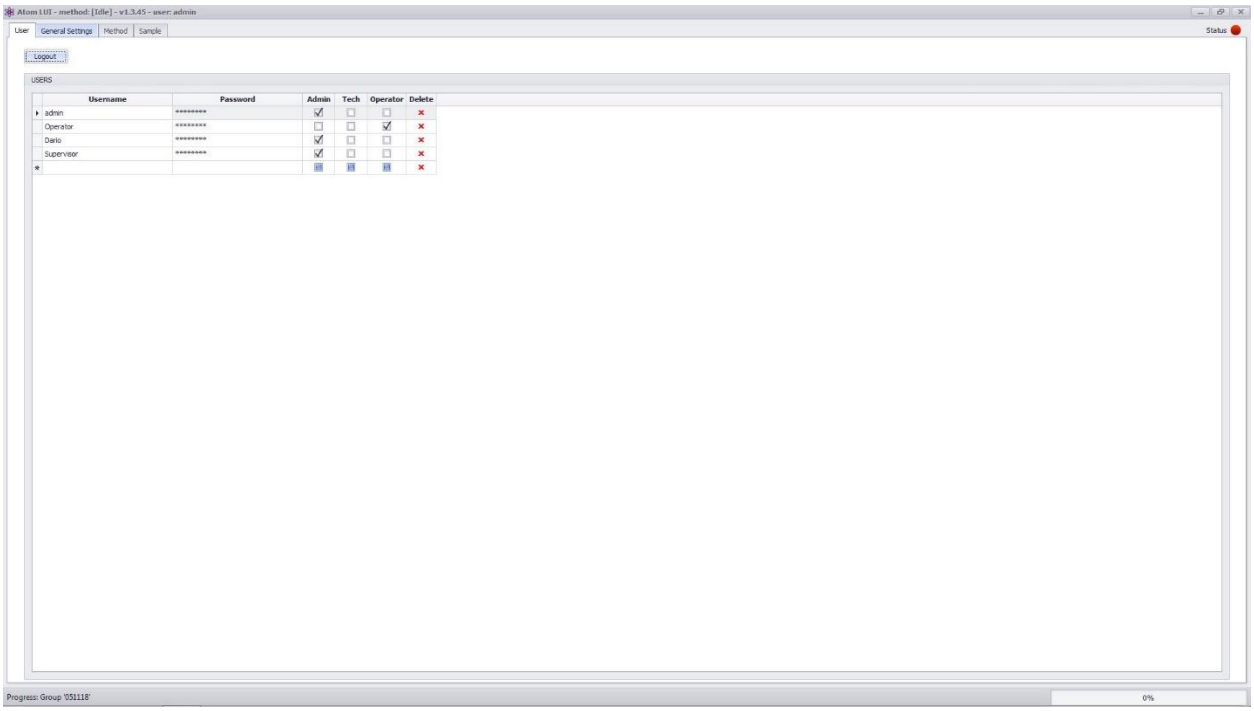


Figure 23 User Tab – Administrator

Section 5.4.2 – Changing Passwords

Section 5.4.2.1 – Administrators

Administrator have full access rights to the XT Series LUI software. Administrator may create new users, change access levels of existing users and change password.

- To add a new user enter the new user in the blank **Username** field, create a **Password** and select the access level by clicking the appropriate checkbox.
- To modify an existing user's access level, click the desired access level for the user.
- To modify an existing user's password (including administrator passwords), enter the new password in the **Password** field
- To delete a user, click the red **x** on the appropriate user's line

Note that the default "admin" user cannot be deleted or modified.

Section 5.4.2.2 – Other Users

Users may modify their password by entering their **Current Password** and typing in the **New Password** in the designated field (Figure 24).

Figure 24 User Tab – Other Users

Section 5.5 – General Settings Tab

The General Settings Tab *(Figure 25)* contains settings relevant to the operation of the LUI.

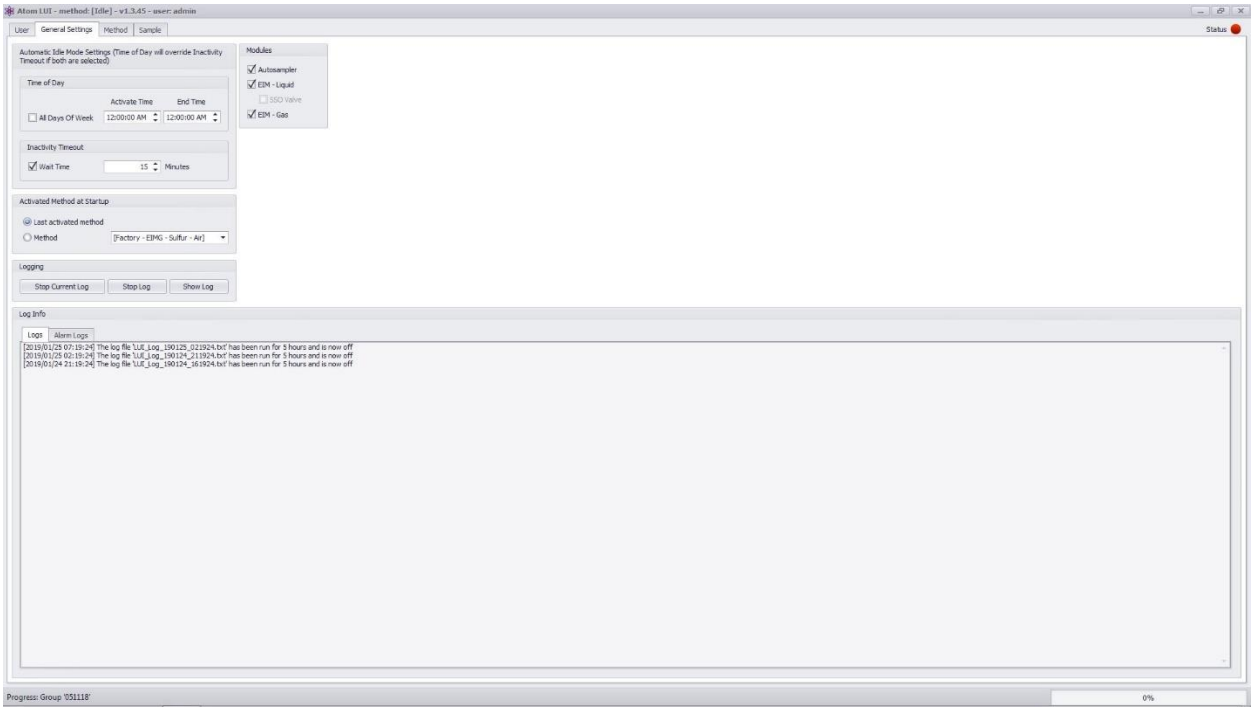


Figure 25 General Settings Tab

Section 5.5.1 – Automatic Idle Method Settings

The LUI features an **Idle Method**, used to reduce consumption of utilities when the analyzer is not in use. The LUI may be set up to automatically activate the Idle Method after a certain period of inactivity (Defined in "**Time After Run Completion**") or during specific periods of the day (Defined in "**Time of Day**"). The Idle Method may be modified as described in Section 5.6 – Method Tab. When the analyzer is shipped, the Idle Method is not automatically set up to activate when the analyzer is not in use. To activate, check the desired checkbox and adjust the corresponding parameters.

Section 5.5.2 – Method Activation Upon Startup

Users may choose which method is automatically activated when the LUI starts up or when the LUI exits Idle Mode. The LUI uses [Factory – AS – Sulfur -Air] Method as default unless changed by a user. The [Factory] methods cannot be modified but may be viewed in the Method Tab, for more information refer to Section 5.6 – Method Tab.

Section 5.5.3 – Logging

For troubleshooting purposes, the LUI features a Logging option. Users may choose to stop the current log file and initiate a new file by clicking the "**Stop Current Log**" button. Users may also choose to stop

logging entirely by clicking the "**Stop Log**" button. Alternatively, users may choose to display the current log by clicking the "**Show Log**" button.

Upon clicking the "**Show Log**" button, a window pops up displaying the current information written to the log file *(Figure 26)*.

Log files are stored in the "**Logs**" folder inside the "ATOM" folder: ATOM/LUI/Logs.

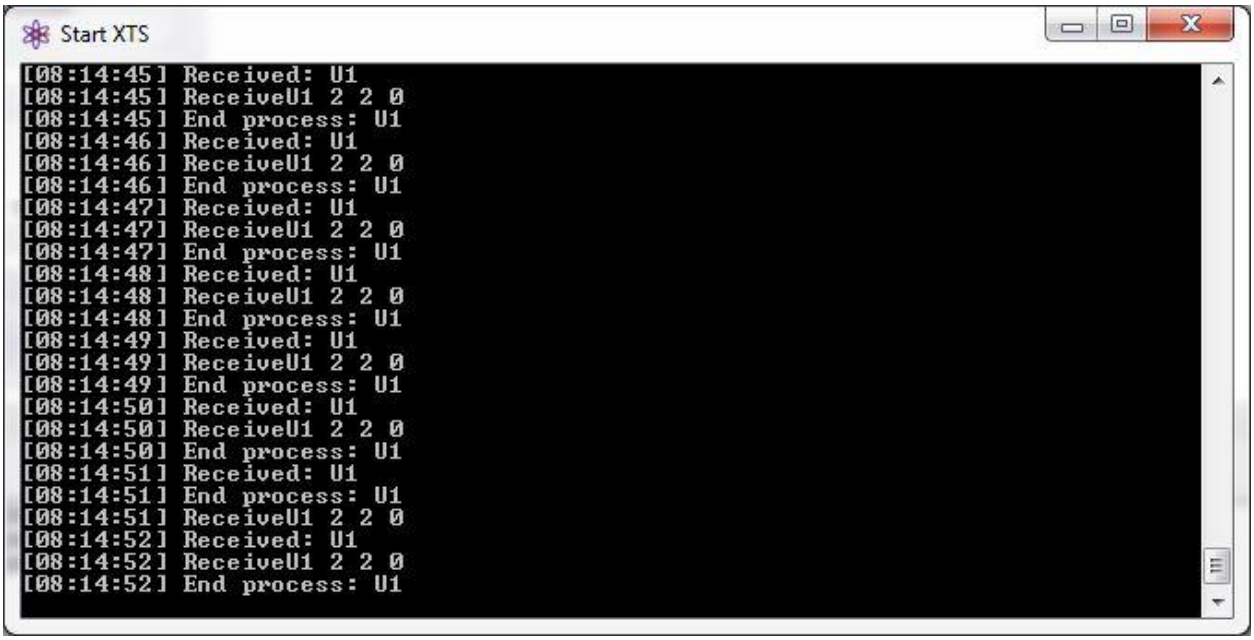


Figure 26 LUI Log

Section 5.5.4 – Log

The bottom section of the General Settings Tab displays log information in two separate tabs: an events log in the first tab and an alarms log in the second tab which details the type of alarm, cause and time of alarm.

Section 5.5.5 – Modules

The Modules section allows users to define which modules are connected to the XT analyzer by clicking the checkbox corresponding to Autosampler, EIM Liquid with or without Sample Shut Off (SSO Valve) and EIM Gas. *Note: The sample shut off valve and gas valve are physically in the same location of the EIM, therefore the user may not select EIM Liquid with SSO Valve and Gas Valve.*

Section 5.6 – Method Tab

The Method Tab *(Figure 27)* is used to define all parameters pertaining to analyses. The Method Tab is divided in two panels. The Method Selection panel on the left displays existing methods by type: Autosampler, EIM-Gas and EIM-Liquid along with the selected method. Users may expand/reduce the left

panel sections for each module by clicking to right corner arrow. The right panel contains a selection of tabs specific to each method.

The ATOM XT Series analyzers come preloaded with multiple methods: [Factory] methods (one for each module and detector combination) and the [Idle] method common to all methods. The Idle method has been previously described in Section 5.5.1 – Automatic Idle Method Settings. The [Factory] methods contain default analysis settings and are not modifiable.

The methods list on the left panel may be exported as a .csv file using the **Export** button. The .csv file contains two columns. The first column corresponds to the Method ID (internal software method number) and the second column includes the name of the corresponding method.

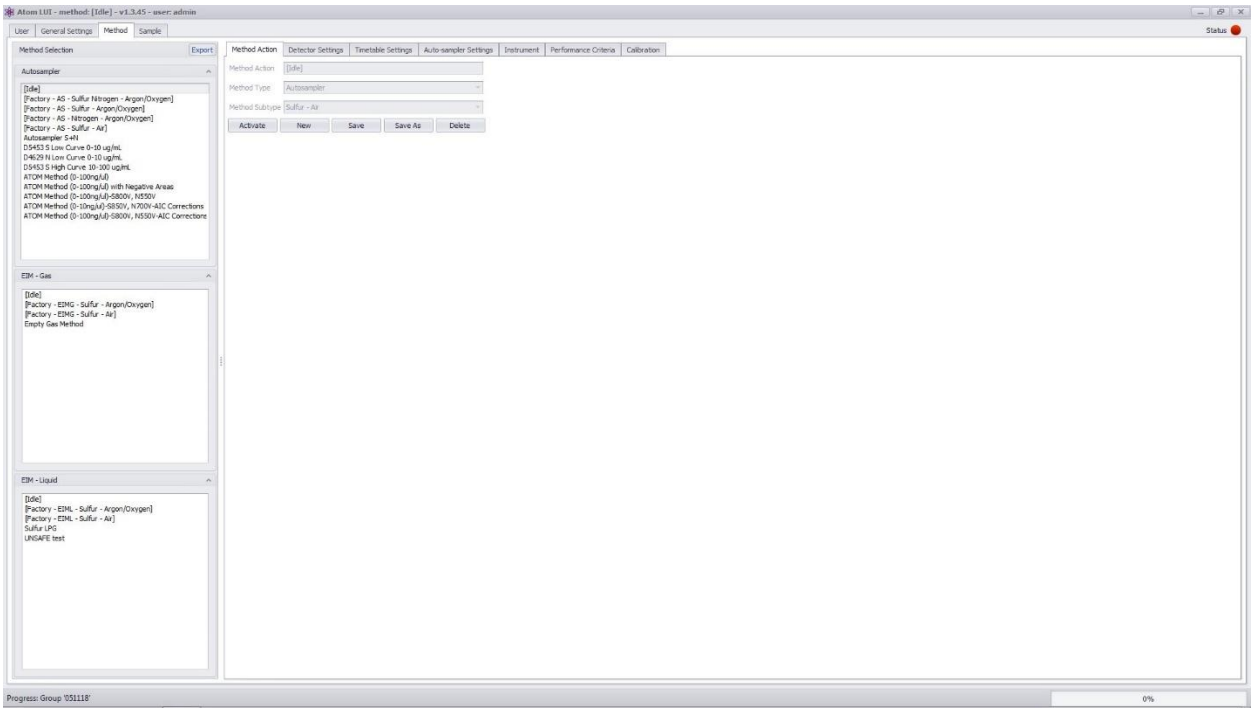


Figure 27 Method Tab and Method Action Tab

Section 5.6.1 – Method Action Tab

The Method Action Tab *(Figure 27)* allows users to create (**New**), **Delete**, **Save**, copy (**Save As**) and **Activate** methods by pressing the corresponding buttons.

Methods are activated in one of two ways: Either by selecting the method of interest in the left panel and clicking the "**Activate**" button, or, by double-clicking on the desired method. To view the activated method, refer to the Status Bar at the top of the screen (See Section 5.2 – Top Bar and Status Button). *Note that double-clicking on a method from any of the Method tabs activates the selected method.*

Methods may be viewed without activation, by selecting the desired method in the left panel. The method currently viewed is highlighted by a grey box.

When running a sample or calibration. The method in use Is colored in blue.

Section 5.6.2 – Detector Settings Tab

Detectors and outputs parameters may be changed through the Detector Settings Tab *(Figure 28)*.

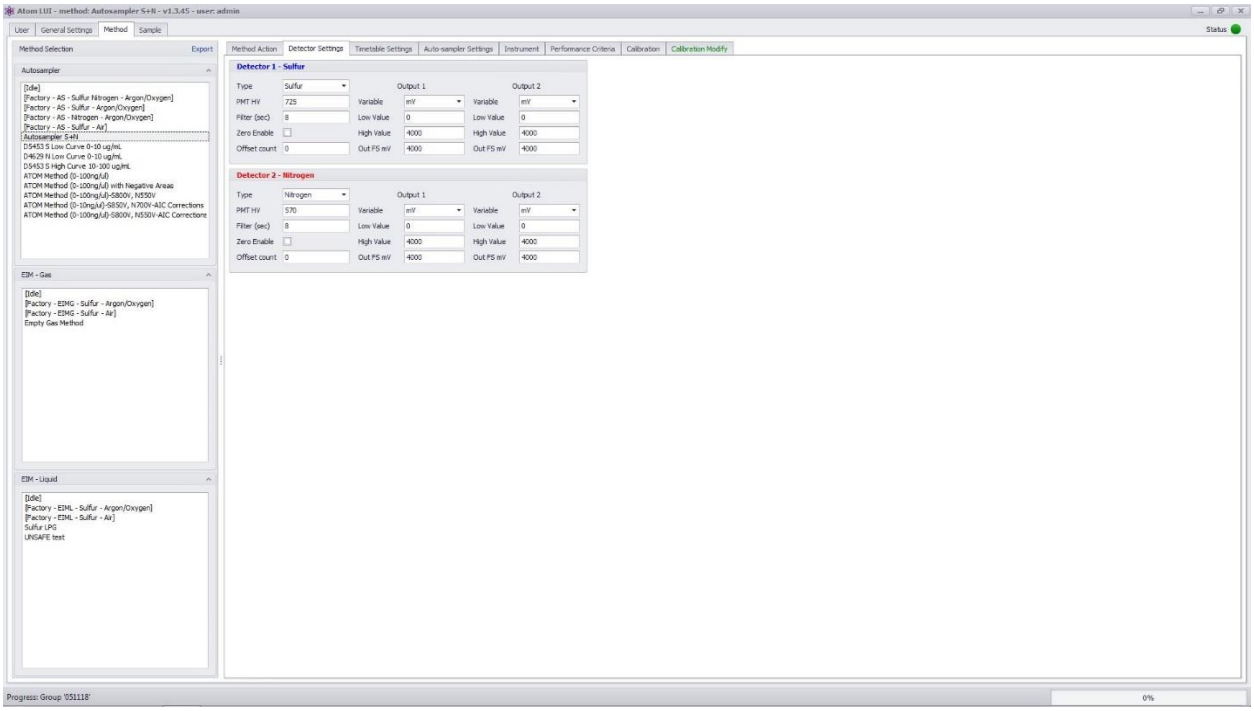


Figure 28 Detector Settings Tab

Section 5.6.2.1 – Detector Settings

The XT Series may be equipped with either Sulfur and/or Nitrogen Detectors, the detector **Type** dropdown menu allows users to choose detector type between Sulfur (Detector 1), Nitrogen (Detector 2) or None.

Detector response can be adjusted by modifying the **PMT HV** input field. Factory default PMT voltage is set by default at 800 V for Detector 1 (Sulfur) and 600 V for Detector 2 (Nitrogen). Note that the maximum allowed PMT voltage is 1099 V.

The **Filter** enables the detector signal to be filtered using a moving boxcar average.. Default factory filter setting is 8 seconds.

For display purposes, users may choose to zero the detector signal. An example of this is to display detector baseline at zero during the analysis. When checked, the **Zero Enable** function sets the analysis baseline at 0. An **Offset Count** ay be added to shift the baseline from 0 in the corresponding field. *Note that the Zero Enable function is for graphical purposes only and has no impact on actual measurement.*

Section 5.6.2.2 – Output Settings

Each detector provides 2 analog **Outputs** . Four variables are available for each output: Detector Signal in microvolts (uV), Detector Signal in millivolts (mV), Base Line (Base Line) or Board Temperature in degrees Celsius (°C), each scalable from 0 to 4V (4,000 mV).

Low and **High** values for each **Output** can be independently set in the corresponding input fields. Low Value and High Value are set for Detector Signal in millivolts (mV) at 0 mV and 4,000 mV.

Section 5.6.3 – Timetable Settings Tab

The XT Series analyze samples cyclically. The analysis cycle is composed of various timed events each defined in the Timetable Settings Tab *(Figure 29)*.

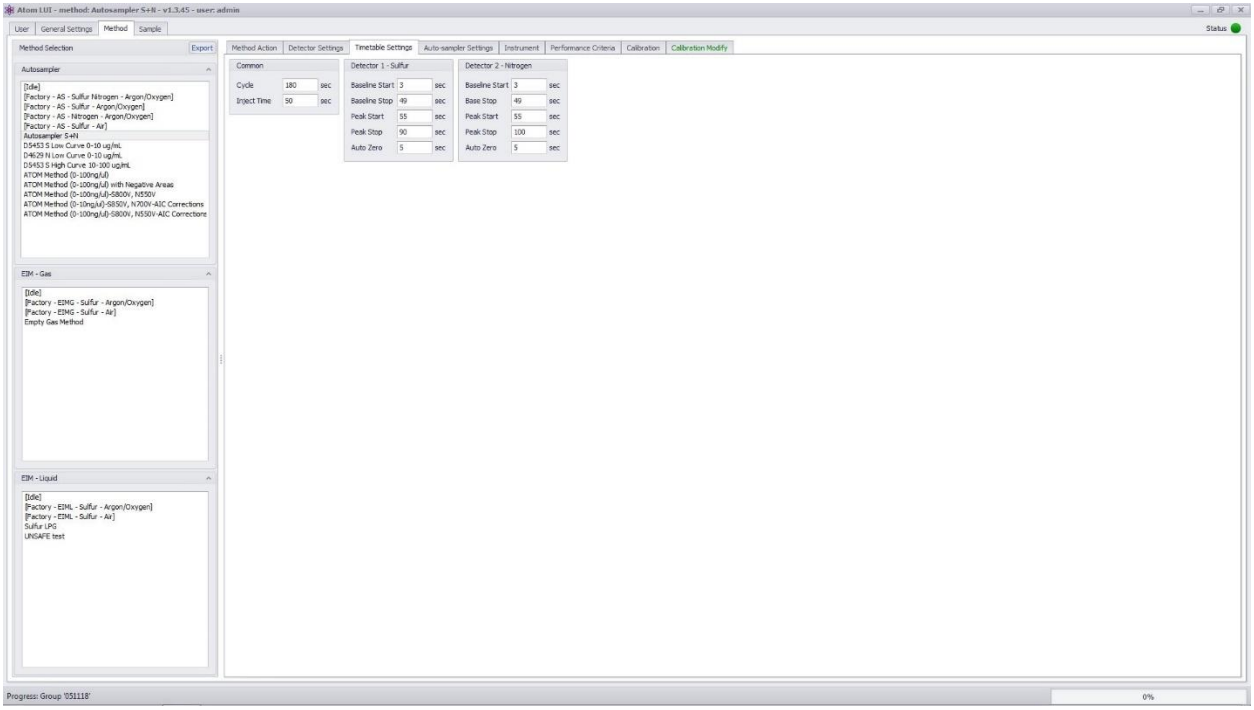


Figure 29 Timetable Settings Tab

The “Common Table” defines events common to both detector: **Cycle Time** and **Inject Time**, both in seconds. Cycle time corresponds to the length of an analysis, set by default at 180s (3 minutes). Inject time corresponds to the time at which the sample is injected in the furnace, set by default at 50s.

Each detector has a timetable where analysis specific events are time defined. For each detector, users may select the **Baseline Start** and **Baseline Stop** time of the baseline evaluation as well as the **Peak Start** and **Peak Stop** time of peak evaluation. For Detector 1, these are set by default at 3s to 49s for baseline evaluation and 55s to 90s for peak evaluation. For Detector 2, these are set by default at 3s to 49s for baseline evaluation and 65s to 110s for peak evaluation. Finally, the **Auto Zero** time determines when the baseline offset will be applied (If Zero Enable function is activated). As described in Section 5.6.2.1 – Detector Settings, users may set the baseline at 0 and offset by a known counts number to visually display a lower baseline.

Section 5.6.4 – Autosampler Settings Tab

When an autosampler is used with the XT analyzer, the Autosampler Settings Tab is used to parameter the autosampler. The autosampler tab is divided into 5 drop-down menus: “Pre Wash”, “Sample Flush”, “Sample”, “Injection”, “Post Wash”. Drop-down menus are arranged in the same order the autosampler uses when preparing a sample.

1) Pre Wash *(Figure 30)*: Sets syringe solvent wash before sample draw. *Please note that pre wash is only performed with a new sample*

2) Sample Flush *(Figure 31)*: Sets syringe sample wash

3) Sample *(Figure 32)*: Sets sample draw

4) Injection *(Figure 33)*: Sets injection parameters

5) Post wash *(Figure 34)*: Sets syringe solvent wash after injection. *Please note that post wash is performed only when changing sample.*

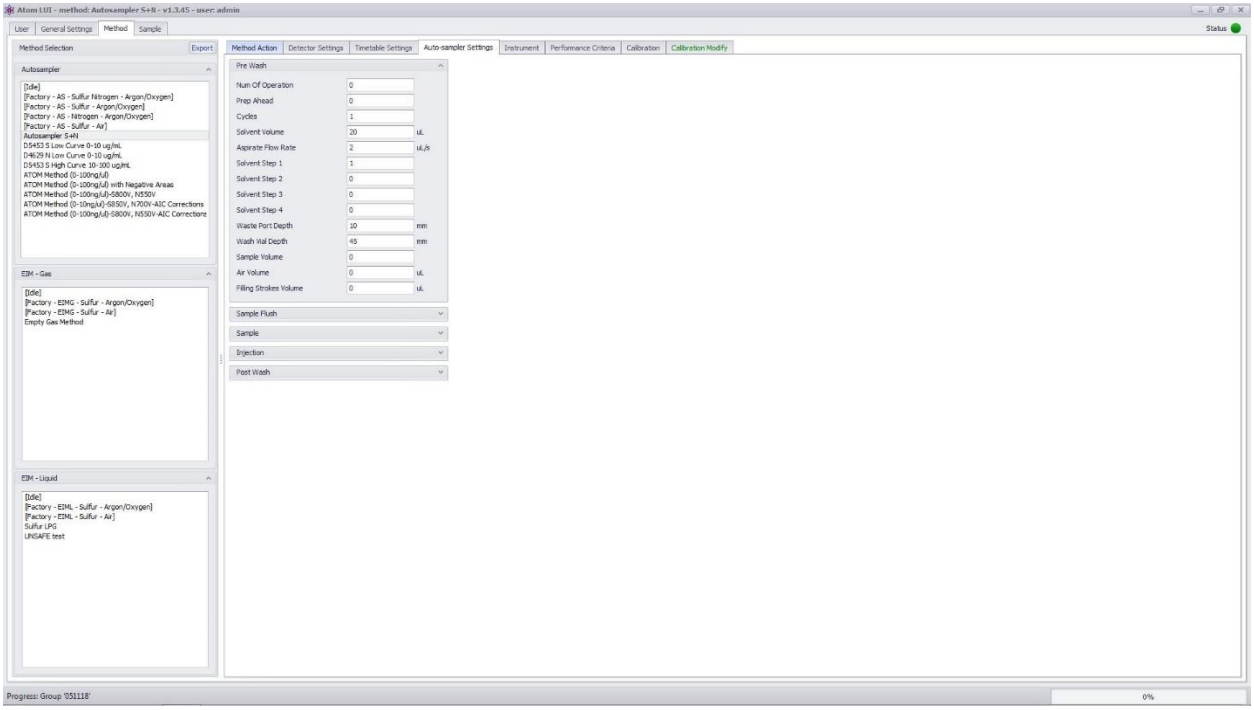


Figure 30 Autosampler Pre Wash Menu

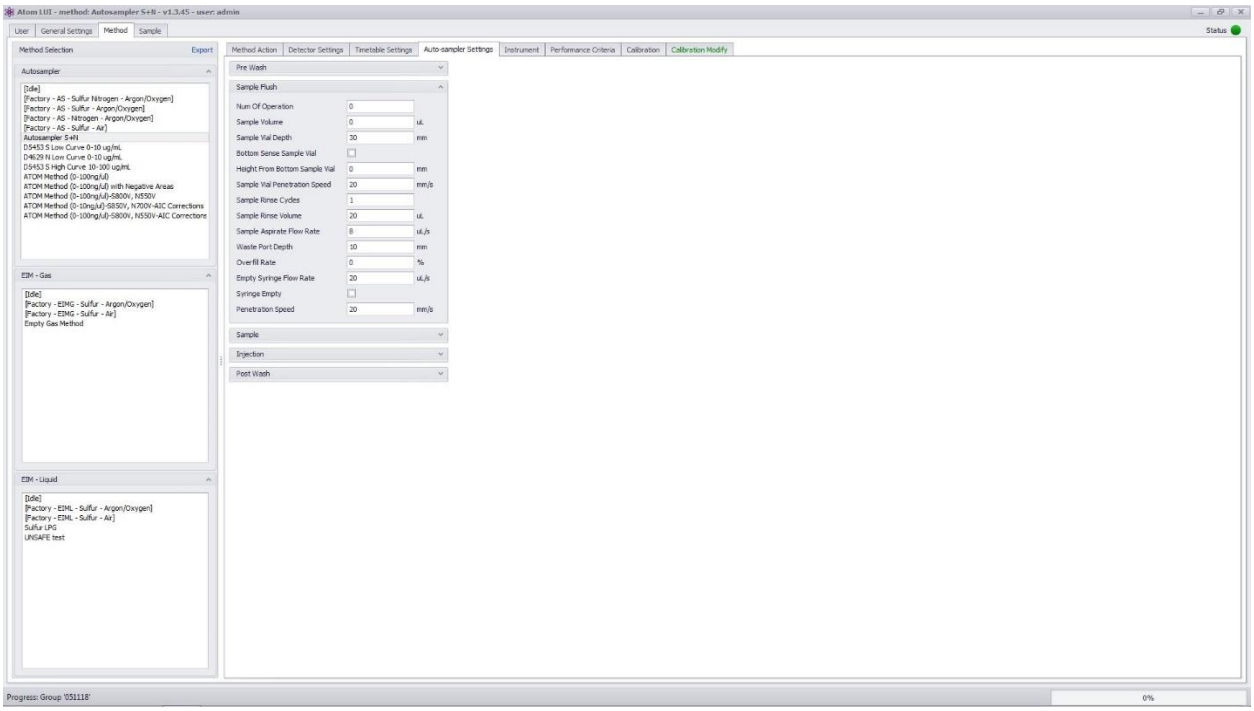


Figure 31 Autosampler Sample Flush Menu

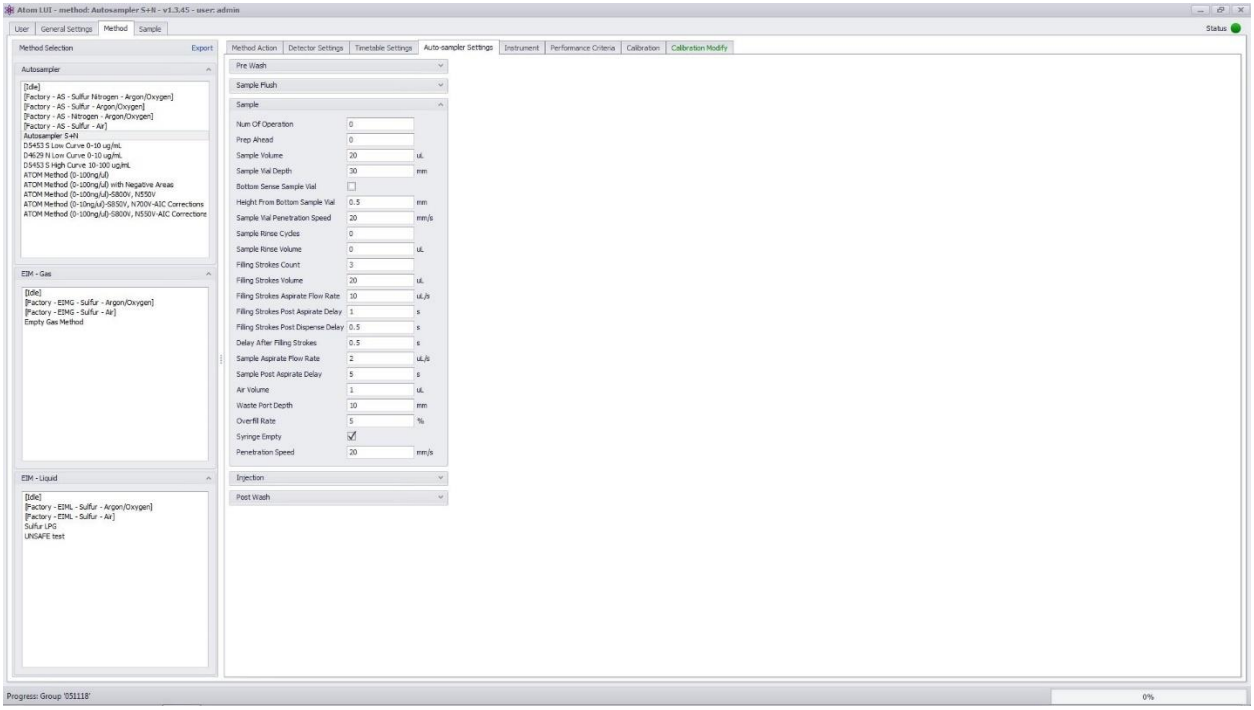


Figure 32 Autosampler Sample Menu

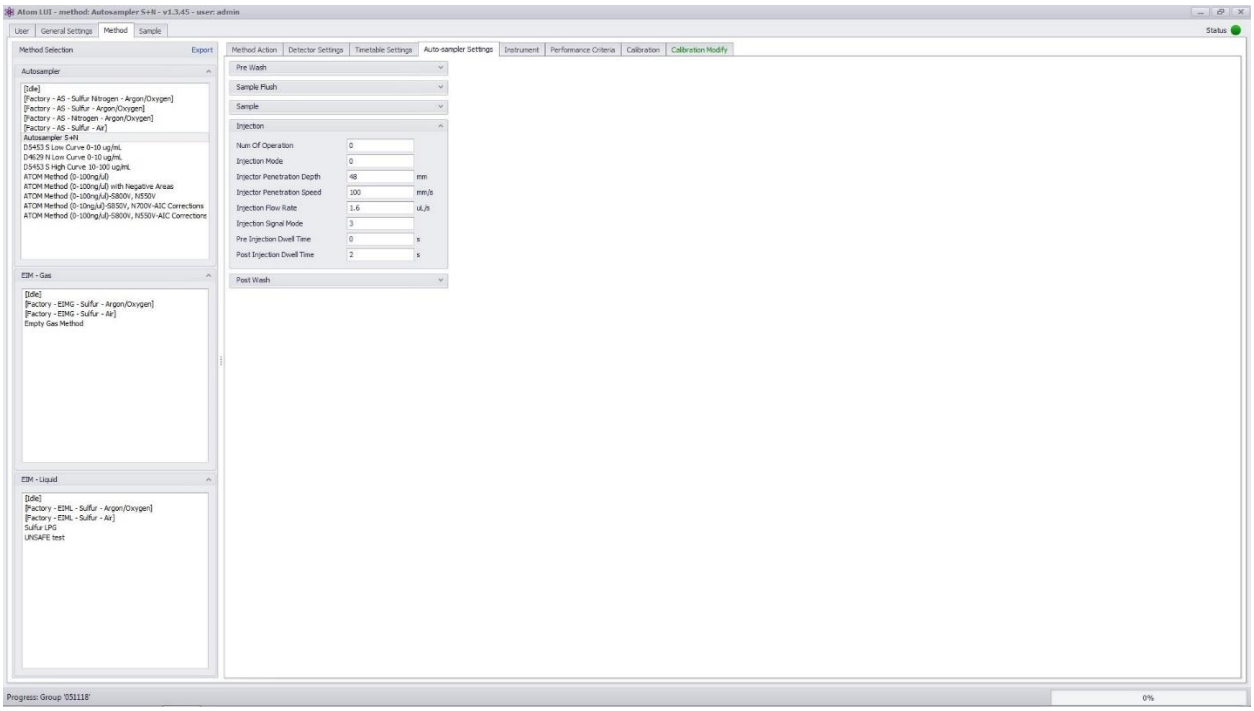


Figure 33 Autosampler Injection Menu

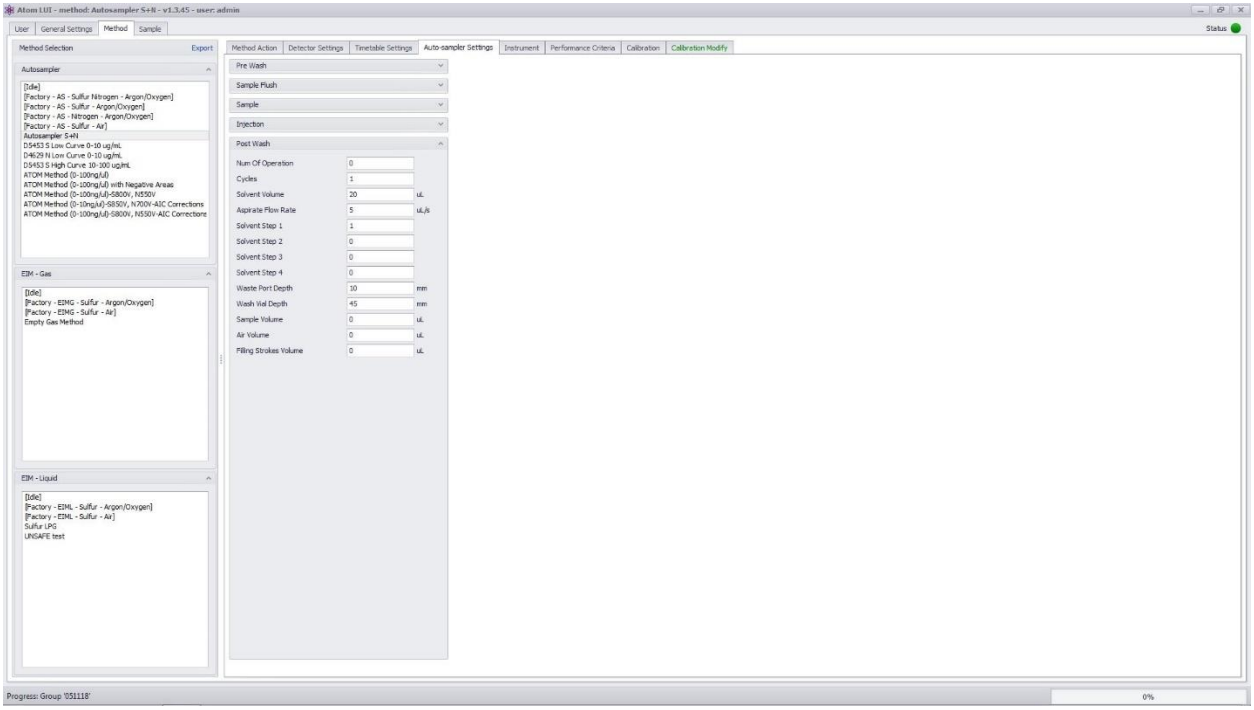


Figure 34 Autosampler Post Wash Menu

Each dropdown menu contains an extensive list of parameters. As most users do not require to modify those parameters to operate the analyzer, only the most relevant parameter of each section are explained

in this manual. For users requiring further assistance with the other parameters, please contact ATOM Instrument or your local agent.

Pre Wash

Cycles: Sets the number of pre wash cycles
Solvent Volume: Sets the volume of solvent drawn in each cycle wash

Sample Flush

Sample Rinse Cycles: Sets the number of wash cycle of the syringe using sample
Sample Rinse Volume: Sets the volume of sample used in each wash

Sample

Sample Volume: Sets the volume of sample that will be injected in the analyzer
Filling Strokes Count: Sets the number of syringe filling/emptying strokes before final draw
Filling Strokes Volume: Sets the volume of each filling/emptying strokes
Sample Post Aspirate Delay: Sets the time delay the autosampler will wait before pulling the syringe out of the sample vial after the sample has been drawn

Injection

Injection Flow Rate: Sets the flow rate (speed) at which the sample is injected

Post wash

Cycles: Sets the number of post wash cycles
Solvent Volume: Sets the volume of solvent drawn in each cycle wash

Section 5.6.5 – EIM Settings Tab

When an External Injection Module (EIM) is connected to the XT, the EIM Settings Tab (Figure 35) is used to parameter the EIM for both liquid and gas samples.

The EIM Settings tab is divided into multiple sections depending on the EIM configuration: Devices, Gas/Liquid Inject Duration, SSO Valve – Analysis Purge and SSO Valve – Status.

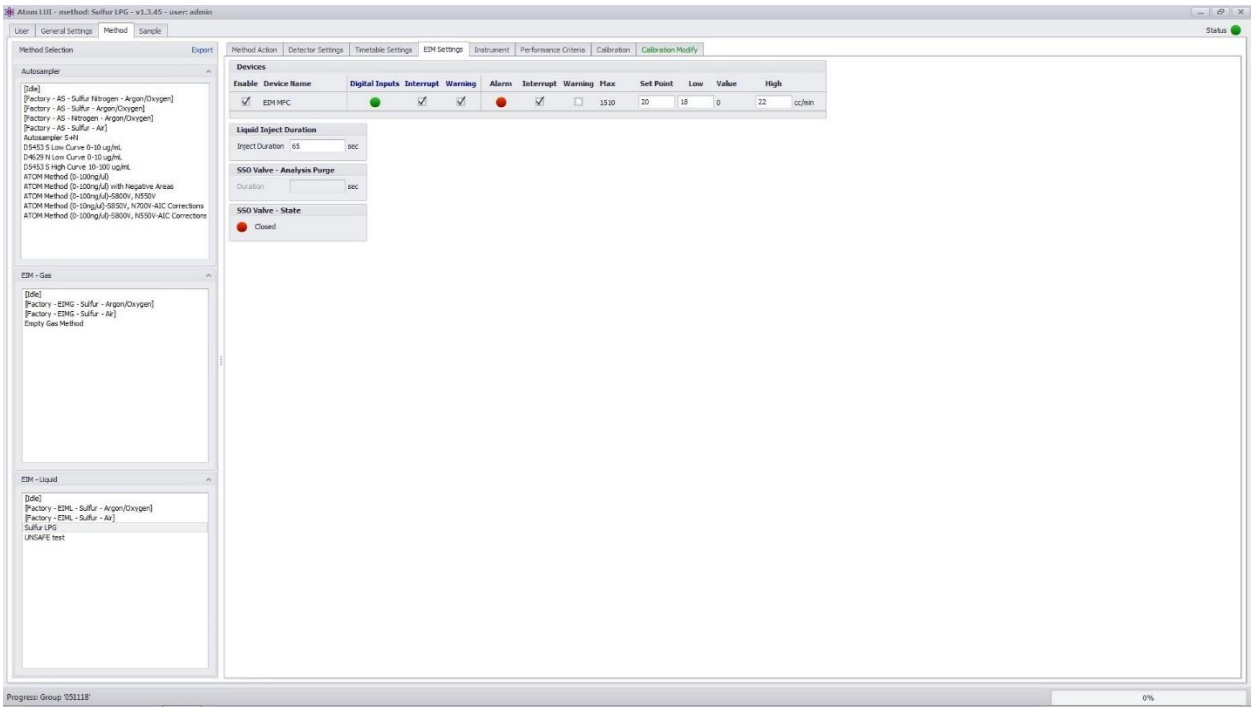


Figure 35 EIM Settings Tab

Section 5.6.5.1 – Devices

Depending on configuration, the EIM can contain a temperature controllers and/or a Mass Flow Controllers (MFC), both commonly called a "device". Each device may be activated and deactivated in this section by clicking the checkbox next to device name.

The temperature controller is used to control the temperature of the gas sample when using a Gas-EIM. The Mass Glow Controller (MFC) is used to set the injection rate of the EIM sample into the XT Series analyzer furnace.

For each device, an associated digital input monitors the status of the device. In case of problem, the analyzer is informed, through the device-specific digital input, of the problem. Users may choose what action is taken if the digital input indicates a problem by either selecting "Interrupt", which stops the analyzer, or "Warning", which displays a warning to users. Radio button indicators are used to display each digital input status: Interrupt 🔴, Warning 🟡, All Clear 🟢.

For each device present (*Note that the Liquid EIM does not use the temperature controller even if present*), users can set the desired **Set Point** (maximum set point value is indicated in the "Max" column) along with **Low** and **High** alarm values and read the real-time value of each activated device in each corresponding column. An alarm state is triggered when the real-time value of the device is outside of the bounds set in **Low** and **High**. When an alarm state is triggered, users may choose what action is taken by the analyzer by either selecting "Interrupt", which stops the analyzer, or "Warning", which displays a warning to users. Radio button indicators are used to display each digital input status: Interrupt 🔴, Warning 🟡, All Clear 🟢

Section 5.6.5.2 – Gas/Liquid Inject Duration

This sections allows the user to choose the gas or liquid valve **Inject Duration**. The default inject duration setting is 65 second. *Note that the maximum inject duration is 65 seconds.*

Section 5.6.5.3 – SSO Valve

When a Sample Shut Off Valve is present in the EIM and the corresponding checkbox is selected in the General Settings tab (Section 5.5 – General Settings Tab), the user may parameter the valve using this section.

Section 5.6.5.3.1 – SSO Valve - Analysis Purge

This section allows users to define an analysis purge. At the beginning of an analysis, the Sample Shut Off (SSO) is deactivated to allow flow through the EIM. Before running a sample, the user is given the choice to purge the system (to ensure that a representative LPG is loaded onto the sample loop) or to run the analysis (For more information, refer to Section 7.4.3 – Liquid Samples With Sample Shut Off (SSO)). The purge time may be edited directly in the SSO Valve - Analysis Purge section. *Note that the minimum purge time is 90 seconds.*

Section 5.6.5.3.2 – SSO Valve State

This section informs the user on the state of the Sample Shut Off. The green radio button corresponds to the SSO valve opened (deactivated) and the red radio button to the SSO valve closed (activated).

Section 5.6.6 – Instrument Tab

The instrument tab *(Figure 36)* is used to set analyzer parameters as well as indicating statuses of the various analyzer components. The tab is divided in five sections: “Devices”, “Detector 1 PMT/Lamp”, “Detector 2 PMT/Lamp”, “Autosampler Status” and “Communication Status”.

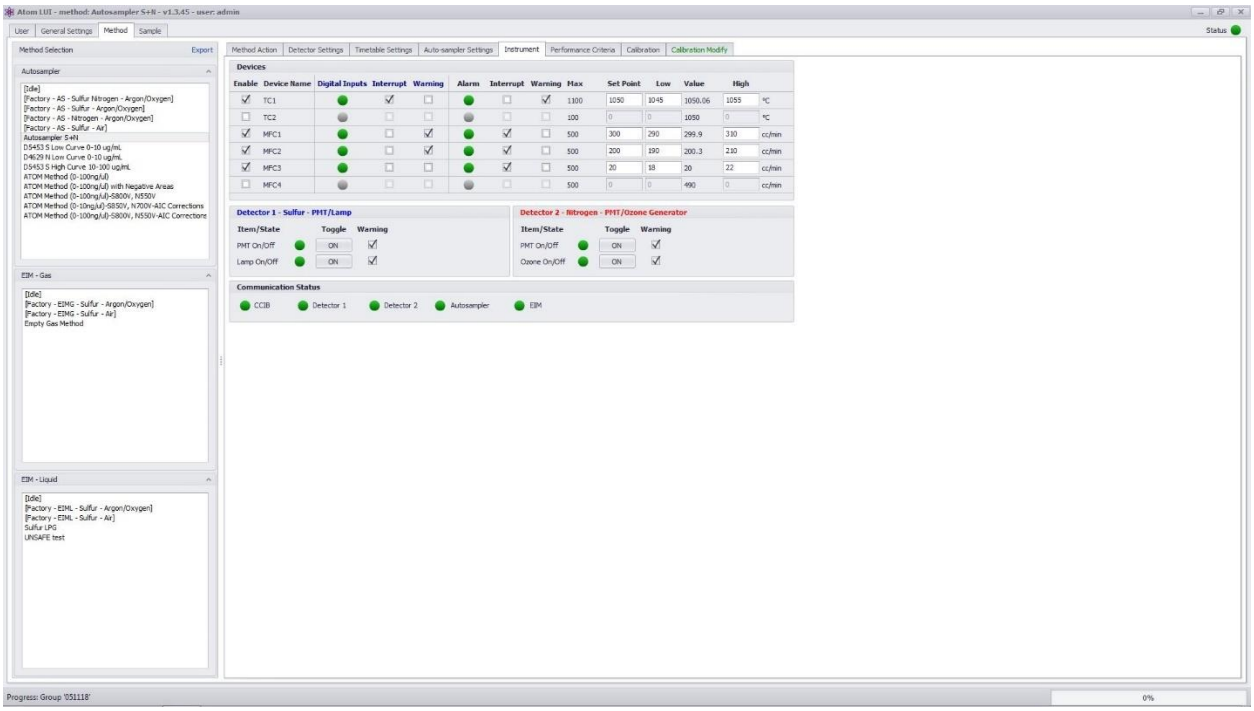


Figure 36 Instrument Tab

Section 5.6.6.1 – Devices

Depending on configuration, the XT Analyzer can contain up to 2 temperature controllers and 4 Mass Flow Controllers (MFC), all commonly called “devices”. Each device may be activated and deactivated in this section by clicking the checkbox next to device name.

Temp1 temperature controller controls the furnace temperature. Temp2 controls the temperature of the dryer (when a heated dryer is installed). MFC1, MFC2 and MFC3 are allocated to oxidizer (air or oxygen), argon and/or oxygen depending on analyzer configuration. MFC4 is currently not in use.

For each device, an associated digital input monitors the status of the device. In case of problem, the analyzer is informed, through the device-specific digital input, of the problem. Users may choose what action is taken if the digital input indicates a problem by either selecting “**Interrupt**”, which stops the analyzer, or “**Warning**”, which displays a warning to users. Radio button indicators are used to display each digital input status: Interrupt, Warning, All Clear.

For each device, users can set the desired **Set Point** (maximum set point value is indicated in the “Max” column) along with **Low** and **High** alarm values and read the real-time **Value** of each activated device in each corresponding column. An alarm state is triggered when the real-time value of the device is outside the bounds set in “Low” and “High”. When an alarm state is triggered, users may choose what action is taken by the analyzer by either selecting “**Interrupt**”, which stops the analyzer, or “**Warning**”, which displays a warning to users. Radio button indicators are used to display each digital input status: Interrupt, Warning, All Clear.

Section 5.6.6.2 – Detector PMT/Lamp-Ozone Generator

For each detector module, users may choose to enable or disable the PMT and/or the lamp/ozone generator by checking the corresponding box. The **Toggle** button allows turning **On** and **Off** the lamp/ozone generator and/or PMT for troubleshooting purposes. *Note that the button displays the current state of the module: ON for on and OFF for off.*
Users may also choose to display a **Warning** if the lamp/ozone generator and/or detector is malfunctioning. Radio buttons are used to display the various possible states of the PMT and lamp: Off 🔴, Warning 🟡, On 🟢.

Section 5.6.6.3 – Communication Status

The XT analyzer has multiple components that do not communicate information through the devices section. Users may know the communication status of the major components: CCIB (Central Communication Interface Board), Detector 1, Detector 2, Autosampler and EIM by looking at the radio button indicators : No Communication 🔴, Communicating with Problems 🟡, Communicating 🟢, Device not Present or Unselected ⚫. When viewing an EIM-Liquid method, an additional radio button “SSO Valve” appears in the list of components to indicate the presence of a sample shut off.

Section 5.6.7 – Performance Criteria Tab

The Performance Criteria tab (Figure 37) allows user to flag samples or runs that do not meet certain criteria. Criteria are detector specific which users may choose to activate on individual runs, on samples (comprised of multiple runs) or both. Users may also choose what the software should do if a sample or run fails to meet the established performance criteria. *Note that performance criteria are specific to each method and may be different from one method to another.*

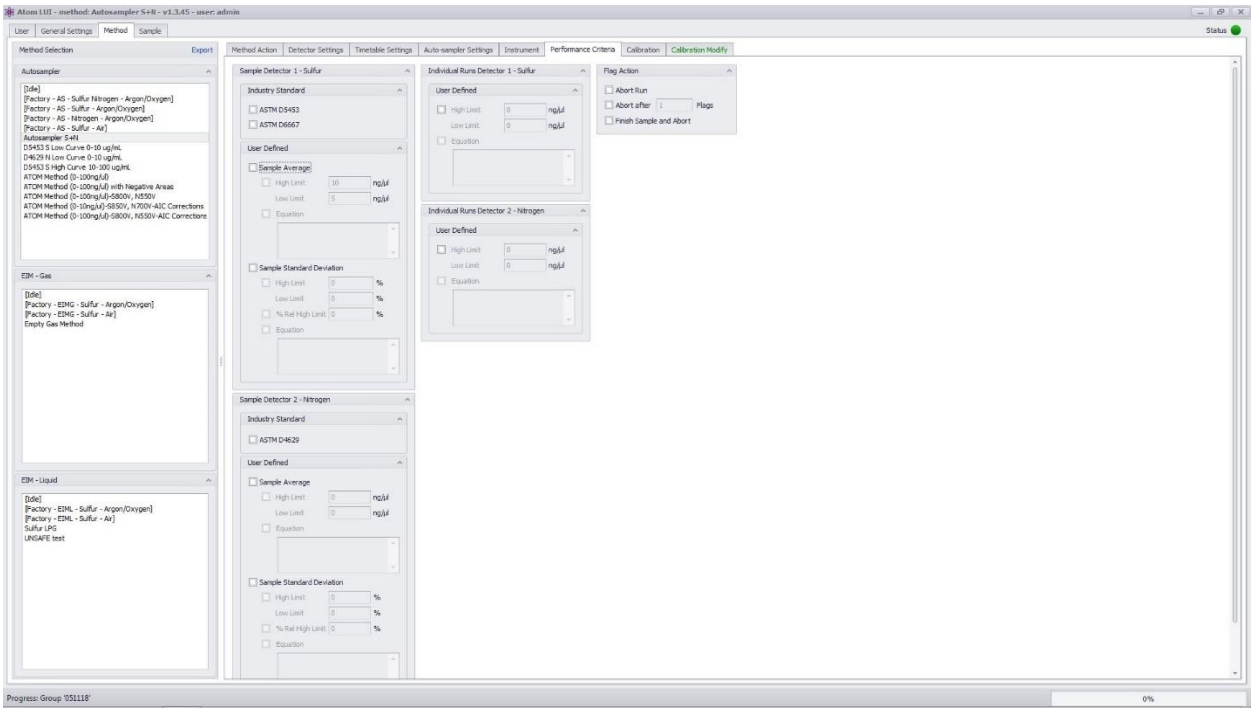


Figure 37 Performance Criteria Tab

Section 5.6.7.1 – Sample Detector 1 – Sample Detector 2

The Sample Detector 1 and Sample Detector 2 dropdown menus allow users to set specific criteria on samples such as those defined by ASTM Standards and/or on the values of the sample average and/or on the relative standard deviation.

Section 5.6.7.1.1 – ASTM Methods

The American Society for Test and Measurements (ASTM) publishes guidelines for the analysis and measurement of a variety of products and processes. One of the subcommittees of the ASTM is dedicated to the measurement of Total Sulfur and Total Nitrogen in hydrocarbon and chemicals. This subcommittee establishes repeatability and reproducibility requirements for equipment measuring Total Sulfur and Total Nitrogen in hydrocarbons and chemicals. The repeatability requirements pertaining to the relevant test methods are built-in the LUI software. These methods include the ASTM D5453, ASTM D6667 and ASTM D4629.

Section 5.6.7.1.2 – User Defined

In this section, users may enter their own requirements on the sample results. Users may set a high and low limit on the sample average concentration and/or a limit on the sample standard deviation. *Note that the equation feature is deactivated at this time. Please reach out to ATOM Instrument if a need appears for this feature.*

Section 5.6.7.2 – Individual Runs Detector 1 – Individual Runs Detector 2

The Individual Runs section allows user to set criteria on the individual runs within a sample. Users may set a high and low limit on individual runs within a sample. *Note that the equation feature is deactivated at this time. Please reach out to ATOM Instrument if a need appears for this feature.*

Section 5.6.7.3 – Flag Action

This section allows users to choose what the system should do once a performance flag has been raised. If no checkbox is selected, the software will flag runs that do not meet the criteria but will not take any action.

Section 5.6.7.3.1 – Abort Run

If the abort run checkbox is selected, the software will abort immediately after the first flag whether on individual runs or sample.

Section 5.6.7.3.2 – Abort after X flags

If the abort after X flags is selected, the software will count the number of flags until it reaches the amount X defined in the input field. Once the amount X of flags is reached, the software will abort the analysis.

Section 5.6.7.3.3 – Finish Sample and Abort

If the Finish Sample and Abort option is selected, the software will finish all the runs in the sample and then abort the analysis.

Section 5.6.8 – Calibration Tab

The calibration tab *(Figure 38)* allows users to associate a calibration to the selected method. Every parameter of the method from the Instrument, Detector Settings, Timetable Settings and Autosampler Settings Tabs will be used when performing the calibration. Once a calibration is associated to a method, it is possible to run samples against this method. For information about running samples, please consult Section 5.7 – Sample Tab.

Each detector activated in the method contains its own tabs. Both detector tabs are laid out identically.

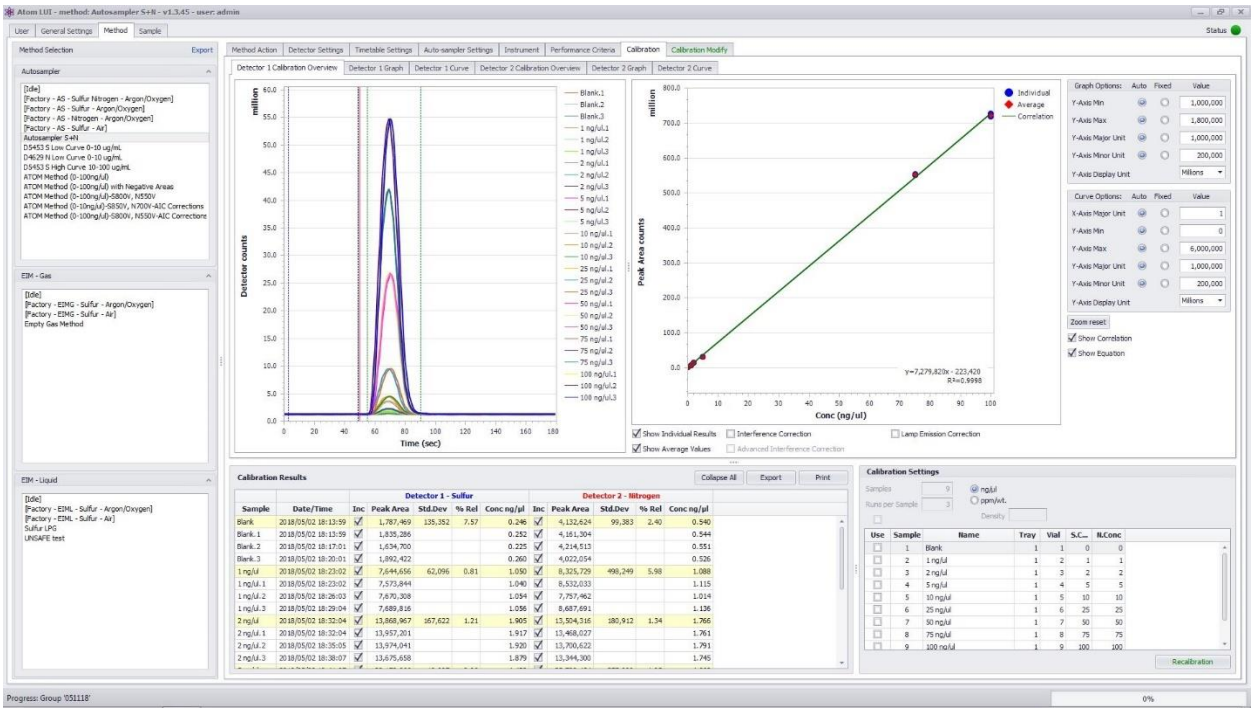


Figure 38 Calibration Overview Tab

Section 5.6.8.1 – Detector Calibration Overview Tab

The Detector Calibration Overview tab *(Figure 38)* is composed of various sections: A section containing a graph, a curve and graphical options, a section with Calibration Results and a section with Calibration Settings.

Section 5.6.8.1.1 – Graph and Curve Area

The graph and curve area contains visual information about the calibration. The graph on the left displays the detector counts vs. time for each individual run contained in the calibration. In the right corner of the

runs graph, each individual run is given a unique color along with a name, based on the sample name inserted in the Calibration Settings Section. All runs are superposed to let users see how each run compares to the others.

The right curve displays the calibration curve of the method along with the equation of the calibration and the coefficient of determination (R^2) correlating the calibration curve with each point included in the calibration. Points in blue represent the peak area of each individual run whereas red points represent the average peak area of each sample used to establish the calibration curve.

Users may modify the graphical properties of the graph or curve by using the options located to the far right. Those options allow modifying axis properties and zoom in/out. Users may also **Zoom In** by holding the Shift button and dragging the mouse over the area of interest or by holding Shift and scrolling with the mouse wheel. The **Zoom Reset** button allows users to return to the original graph/curve magnification.

Below the curve area, various checkbox give access to further graphical parameters for the calibration curve only. A parameter is selected by checking the checkbox next to it. **Show Individual Results** displays blue points corresponding to the peak area of each individual run in the calibration. **Show Average Values** displays a red point corresponding to the average peak area of all the runs included in a standard. **Show Correlation** and **Show Equation** display the equation and coefficient of determination (R^2) of the calibration curve.

Interference Correction, **Advanced Interference Correction** and **Lamp Emission Correction** are not calibration curve graphical settings but calibration parameters that modify the calibration behavior. **Interference Correction** forces the calibration curve to pass through the (0;0) point by removing the y-axis intercept of the calibration. The **Advanced Interference Correction** is a secondary correction enabled once the standard Interference Correction has been activated. The **Advanced Interference Correction** offsets the calibration curve to force it to pass through the lowest concentration point of the calibration (usually a low value blank). *Note that Interference Correction and Advanced Interference Correction are detector specific and must be activated separately for each detector.* **Lamp Emission Correction** is a drift correction to account for the decay of lamp intensity and its impact on measurement. This setting must be activated before calibration for it to be accounted for afterwards.

Section 5.6.8.1.2 – Calibration Results

This section displays the numerical results of the calibration in the form of a table. For each sample defined in the Calibration Settings section, average and individual run information is given. The average sample results are highlighted in yellow with each run included in the average displayed below the average.

The name of each individual run corresponds to the sample name followed by the run number. **Sample Name** and **Date and Time** at which each run was performed are displayed in the corresponding columns. **Peak area** and **Calculated Concentration** are also given for each individual run.

The **Sample Average**, highlighted in yellow, displays the same type of information as each individual run but also includes statistical data in the form of **Standard Deviation** of the peak area and **Relative Standard Deviation** (%rel) to the average.

For each run, users may choose to include or exclude a run from the average by checking the corresponding box in the "Inc" column. Users may also **Collapse/Expand All** to display only the average result per sample or all the runs included in the calibration sample.

The **Export** button allows exporting calibration data to a .csv file for further treatment. Users may choose to export the **Summary** of the calibration which includes the settings of the calibration along with the information displayed in the calibration table, **Details** of the calibration which include the detector counts over time used to create the graphs, or both.

Users may also print the calibration results. When clicking on the **Print** button, a separate window opens giving users access to a print preview and the options to change background color, put a watermark, export the calibration in pdf form and e-mail the calibration.

Section 5.6.8.1.3 – Calibration Settings

Calibration parameters are located in the **Calibration Settings** section. To perform a calibration, users must first specify in the corresponding input spaces: the **Number of Samples** in the calibration, how many **Runs per Sample**, the concentration **Unit** of the samples and if ppm/wt is selected, the **Density** of the samples.

After specifying the information general to all samples, users must then enter the sample-specific information in the corresponding table. For each sample, users must enter the **Name** and **Concentration** of the sample. The Concentration field is specific to each detector type (Sulfur: S.Conc and Nitrogen: N.Conc) and the corresponding field will appear depending on the detector selected in Detector Settings Tab (Section 5.6.2 – Detector Settings Tab) If using an Autosampler, users also need to specify the **Tray** and **Vial Number** corresponding to each sample. If using an External Injection Module, the tray and vial boxes are greyed out.

Once all the information is entered in the Calibration Settings section, the calibration is started by pressing the "**Run**" button. Users may track the progress of the calibration by monitoring the progress bar at the bottom right of the LUI. The LUI will also highlight the sample currently in use in the calibration.

Note that when calibrating an EIM method, the software will prompt the user to switch from one standard to the other.

Section 5.6.8.2 – Detector Graph Tab and Detector Curve Tab

The **Detector Graph** Tab *(Figure 39)* and **Detector Curve** Tab *(Figure 40)* contain enlarged versions of the corresponding graph and curve encountered in the Detector Calibration Overview Tab. Users may do the same graphical modifications as in the Detector Calibration Overview Tab using the right hand graphical parameters and checkboxes.

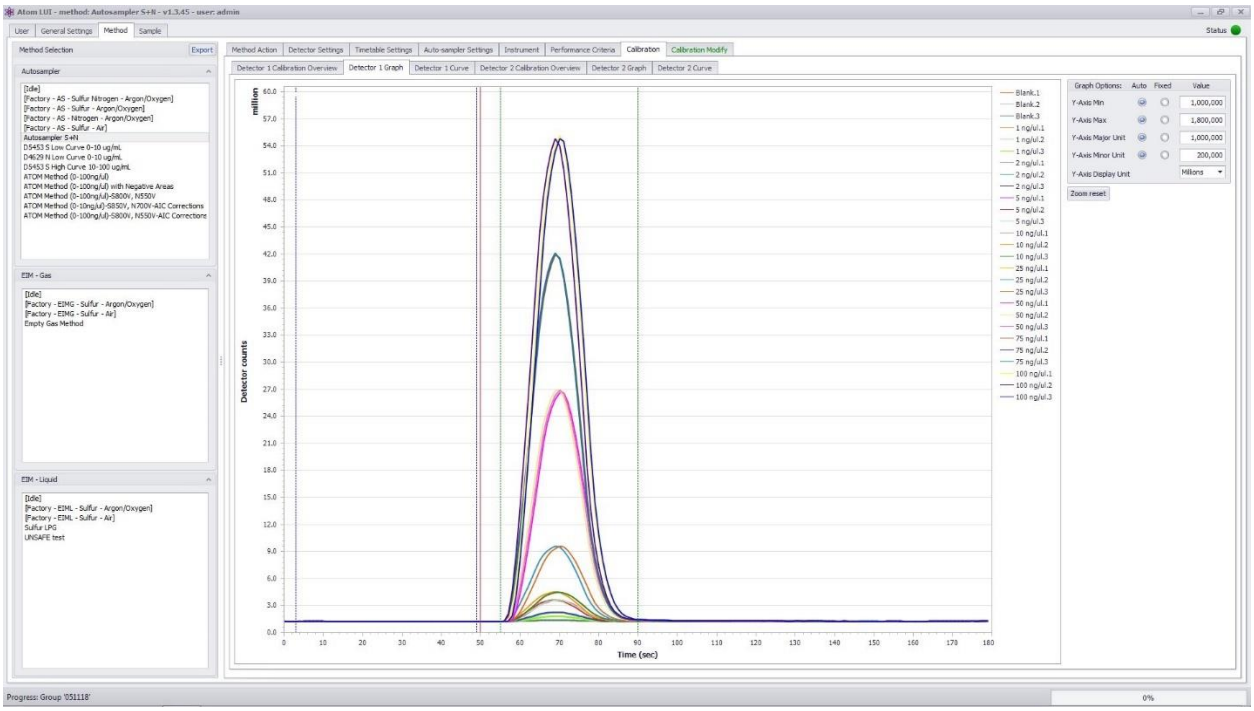


Figure 39 Detector Graph Tab

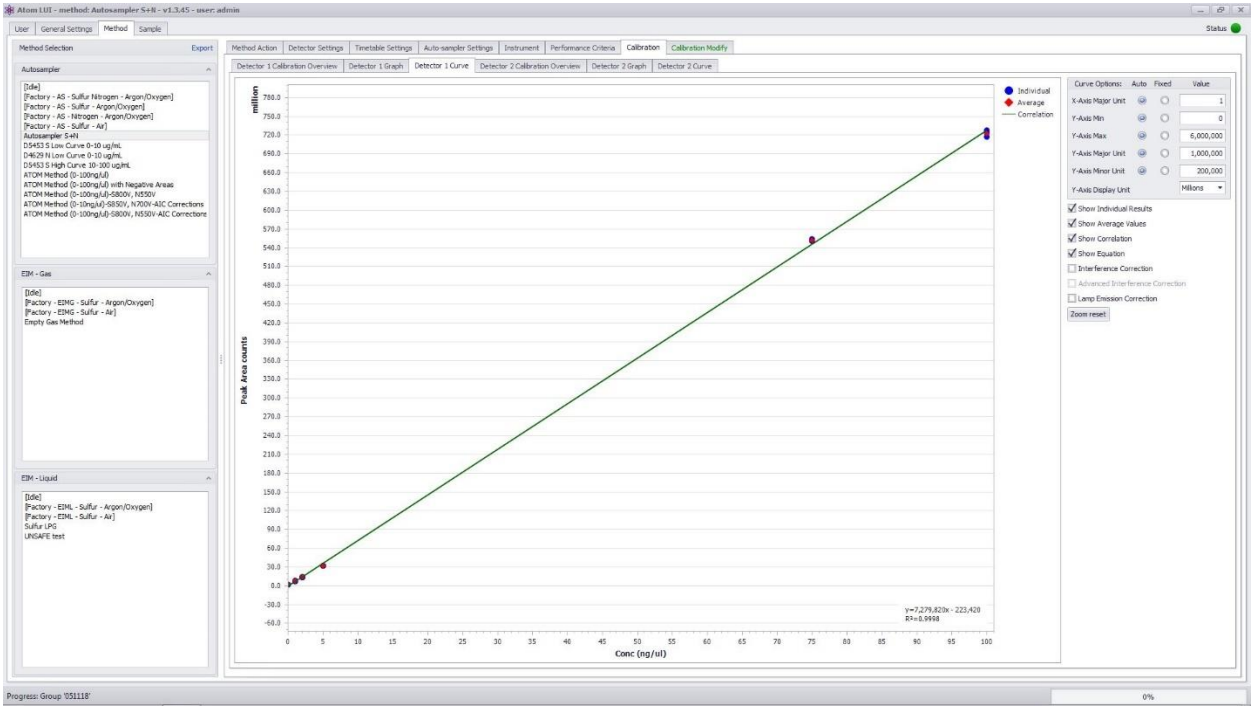


Figure 40 Detector Curve Tab

Section 5.6.9 – Recalibration Tab

Once a calibration is complete, users may recalibrate the method by pressing the **Recalibration** button. Upon pressing the button, a separate tab called Recalibration appears *(Figure 41)*. The Recalibration tab includes the same tabs as the Calibration tab: Detector Calibration Overview, Detector Graph and Detector Curve tabs which retain the same functionalities. Users may change the desired parameters and/or calibration settings before starting a new calibration. The recalibration starts when the user presses the "**Recalibration**" button.

Once the recalibration is finished, users may choose to save the new calibration by pressing the **Save** button. The LUI will keep in memory the new calibration when switching tabs so that users may compare the new calibration with the old calibration before saving the new calibration.

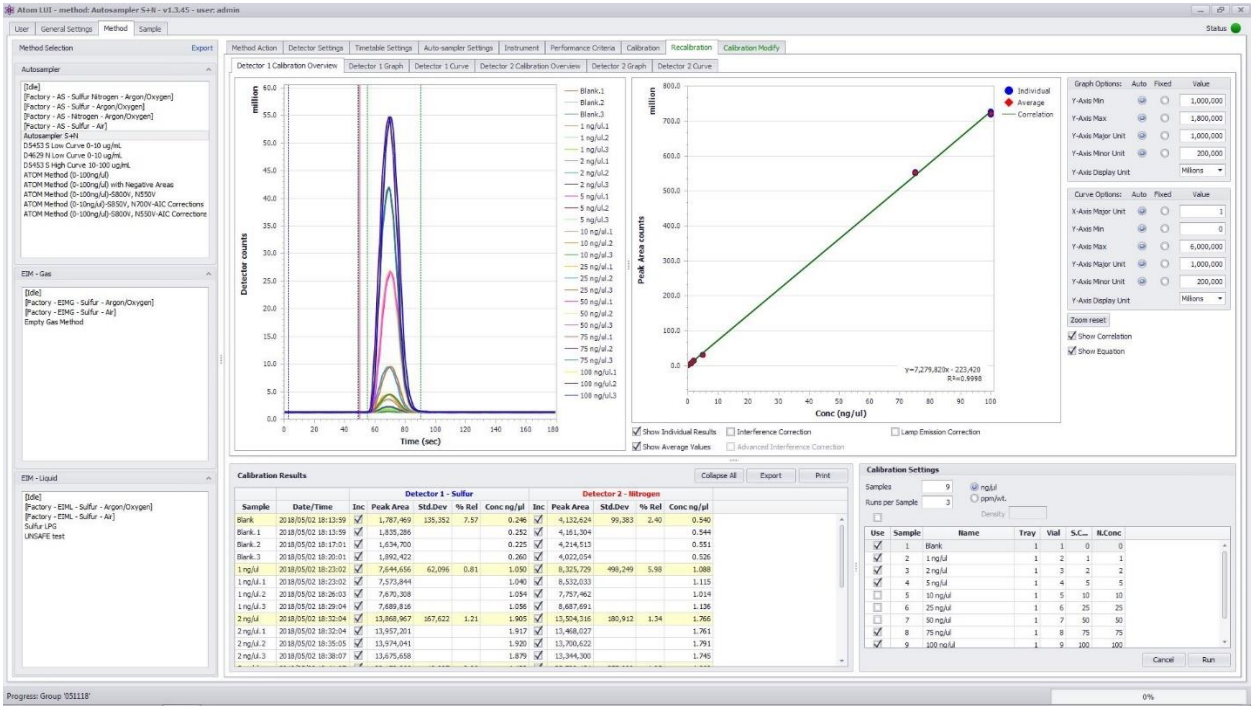


Figure 41 Recalibration Tab

Section 5.6.10 – Timetable Modify Tab

Once a calibration has been established for a method, the **Timetable Modify** Tab will appear *(Figure 42)*, allowing for calibration recomputation. The Timetable Modify Tab allows users to modify a calibration without having to do a recalibration. Since the recomputation feature does not perform any measurement on samples but rather modifies mathematically the calibration, some of the calibration parameters may not be changed. The Timetable Modify tab contains two tabs: Timetable and Calibration.

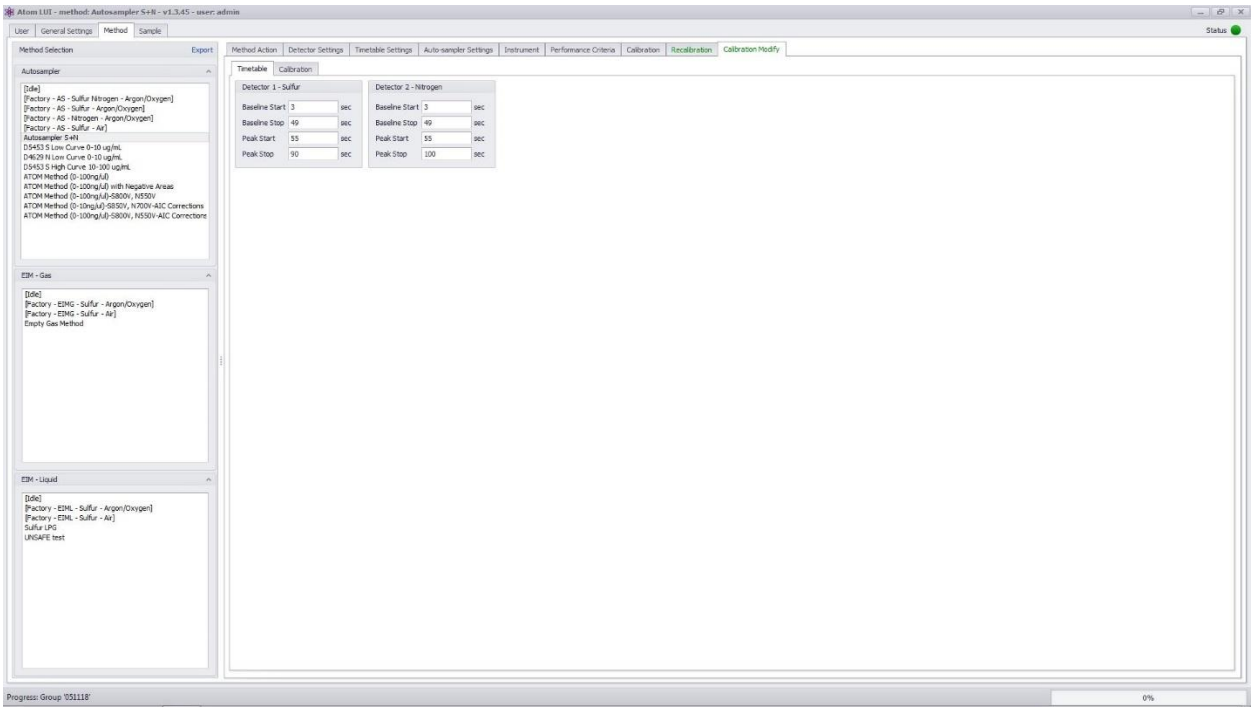


Figure 42 Timetable Modify Tab

Section 5.6.10.1 – Timetable Tab

The Timetable tab *(Figure 42)* allows users to modify detector specific timetable settings but not common parameters such as injection time or cycle time.

Section 5.6.10.2 – Calibration Tab

The Calibration Tab *(Figure 43)* contains the same tabs as the main Calibration Tab: Detector Calibration Overview, Detector Graph and Detector Curve.

Parameters that may be recomputed in the Timetable Modify Tab include the following:

- Selection of individual runs included in the calibration. *Note, runs may only be removed.*
- Samples included in the calibration. *Note, samples may only be removed.*
- Concentration of the samples
- Names of the samples

Once users have modified the desired parameters, either in the Timetable Tab or the Calibration Tab, the "**Recompute**" button appears. By clicking the Recompute button, the LUI will recalculate the new calibration based on the modified parameters.

Users may choose to save the recomputed calibration by pressing "**Save**" or discard it by pressing "**Reset**". The LUI will keep in memory the recomputed calibration when switching tabs so that users may compare the recomputed calibration with the current calibration before saving the recomputed calibration.

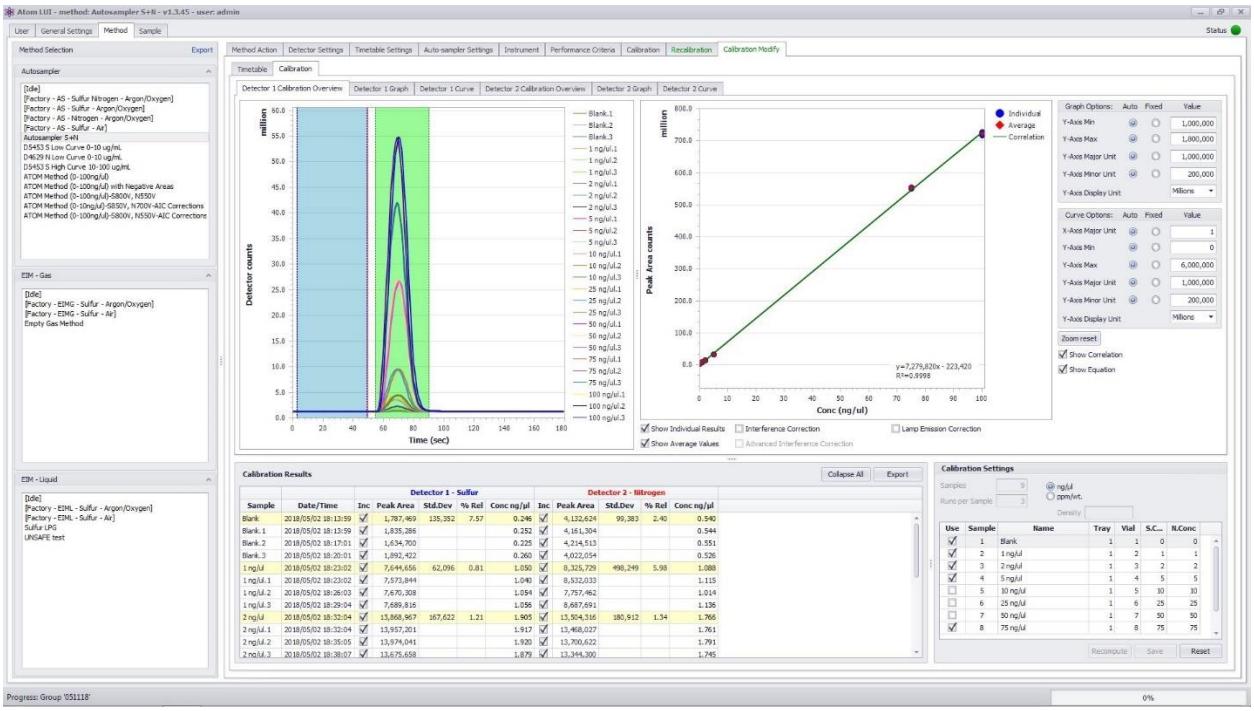


Figure 43 Calibration Tab

Section 5.7 – Sample Tab

The sample tab *(Figure 44)* allows users to run samples against calibrated methods to measure the total sulfur and/or total nitrogen content of samples. The sample tab is divided into various sections: The left pane along with the top bar contain information about groups whereas the graphs section, the Sample Results Section and Sample Settings section contain information specific to samples.

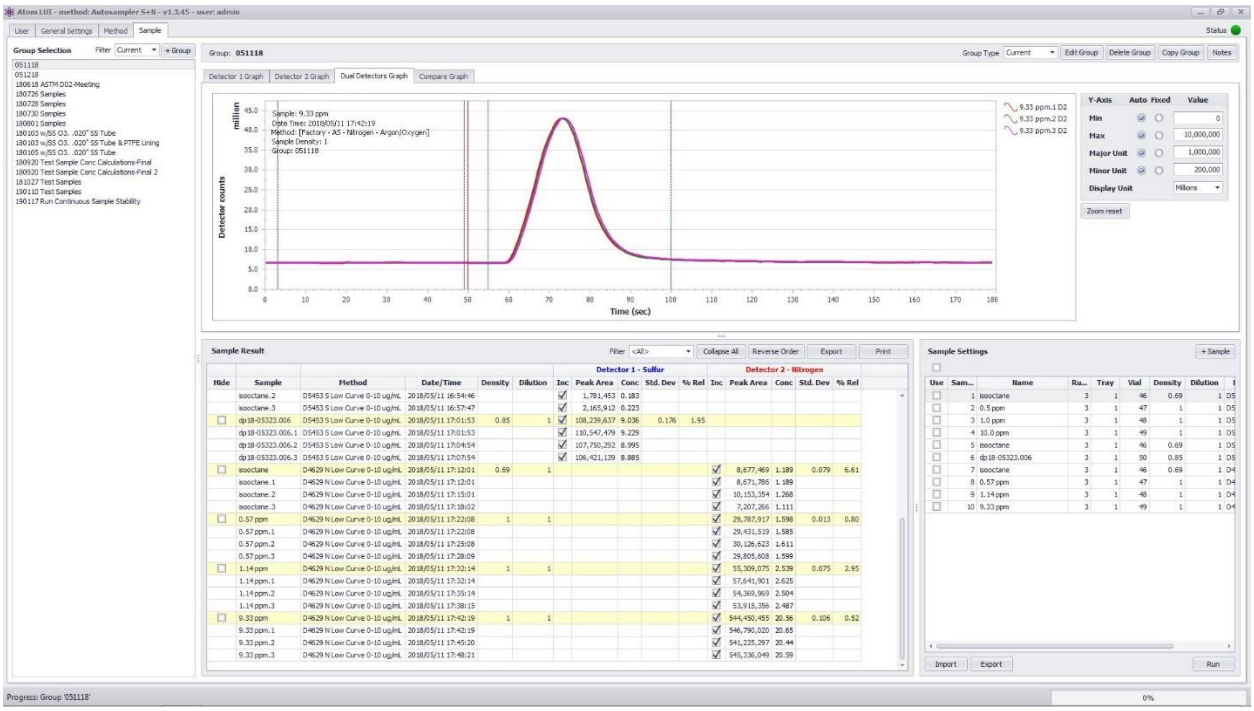


Figure 44 Sample Tab

Section 5.7.1 – Sample Groups

To be analyzed, samples must be part of a group. A group may contain various samples and a sample may be present in various groups. To create a group users must click the **"+ Group**" button. Upon clicking the + Group button, the "**Create New Group**" window will appear.

The Create New Group window allows naming the newly formed group as well as putting notes pertaining to the group. The group may be created without any samples by selecting the "**Create group to run new samples**" radio button or may include runs from other groups.

If "**Create group from existing sample sets**" is chosen, users may select in the "**Sample set list**" dropdown menu samples from which groups will be used. To select a sample to include in the new group, users must check the checkbox corresponding to the desired sample and press the corresponding green arrow to include the checked samples in the "**Selected sample sets**". Users may also remove samples from the Selected sample sets by checking the corresponding checkboxes and clicking the corresponding green arrow.

Users may also choose to duplicate entirely an existing group by selecting the "**Duplicate another group**" radio button. Upon selecting this radio button, the list of existing methods to choose from will appear in the "**Group Selection**" window.

Upon creation, the new group will appear in the left pane at the bottom of the list.

Section 5.7.1.1 – Group Status Bar

The Group Status bar at the top of the sample tab contains information and actions relevant to a specific group. The group currently selected is highlighted in grey in the Group Selection pane.

The group name is displayed in bold to the left of the Status bar. Various group-specific actions buttons are present to the right of the status bar:

- Group Type: Groups mays be **Current** or **Archive**. Users may change group type by selecting the corresponding option in the "**Group Type**" drop-down menu. A Current group may be Archived and vice-versa.

  To display archived groups, users must select "Archive" in the Filter drop-down menu in the Group Selection pane to the left of the screen.

- Edit Group: Groups may be edited after they are created. Upon clicking "**Edit Group**", the Edit group window opens. Users may then **Rename** the group, insert **Notes** and **Add/Remove** samples. To add/remove samples to the new group, users must check the checkbox corresponding to the desired sample and press the corresponding green arrow to add/remove the checked samples in the "**Selected sample sets**". Users may choose to add samples from a specific group by choosing the desired group in the Group Filter drop-down menu.

- Delete Group: Allows users to **Delete** a group. **WARNING: Deleting a group will delete all samples that are not included in another group.**

- Copy Group: Copying a group will **Copy** all samples and parameters entered in the group. Upon clicking "Copy Group" users are prompted to enter the name of the copied group. *Please note that multiple groups may have the same name.*

- Notes: Groups can be created/edited with **Notes**. Clicking the "Notes" button shows the notes specific to the group for users to view/edit.

Section 5.7.1.2 – Group Selection Pane

The left pane of the Sample tab contains all the groups saved in the database. Groups may be either "Current" or "Archive". Users may switch between current and archived groups, by selecting the corresponding filter in the **Filter** drop-down menu.

The group currently in view is highlighted in grey. *Please note that only one group may be selected for view at a time.*

Section 5.7.2 – Graph area

The Graph area contains visual information about the analyzed sample. The graph displays detector counts vs. time plot for each individual run contained in the sample. To the right side of the runs graph, each individual run is given a unique color along with a name, based on the sample name inserted in the Sample Settings Section. All runs are superposed to let users see how each run compares to the others.

Users may choose to display the detector counts vs. time plot for a specific detector or for both sensors simultaneously by selecting the corresponding tab.

Users may modify the graphical properties of the graph by using the options located to the right. Those options allow modifying axis properties and **Zoom In/Out**. Users may also zoom in by holding the Shift button and dragging the mouse over the area of interest or by holding Shift and scrolling with the mouse wheel. The Zoom Reset button allows users to return to the original graph/curve magnification.

Section 5.7.3 – Sample Results

This section displays the numerical results of the analyzed samples in the form of a table. For each sample defined in the Sample Settings section, average and individual run information is given. The **Average** sample results are highlighted in yellow with each run included in the average displayed below the average. The name of each individual run corresponds to the sample name followed by the run number.

For each run, the **Method** used to analyze the sample, the **Date and Time** at which each run was performed and the **Density** of the sample (when using a method calibrated in ppm/wt) are given in the corresponding columns. Detector specific information: peak area and calculated concentration, are given in corresponding columns for each detector.

The sample average, highlighted in yellow, will display additional runs information in the form of statistical data: **Standard Deviation** of the peak area and **Relative Standard Deviation** (%rel) to the average, both displayed in corresponding column for each detector.

For each run, users may choose to **Include** or **Exclude** a run from the average by checking the corresponding box in the “Inc” column. Users may also **Collapse/Expand All** to show only the average result per sample or all the runs included in the sample.

The **Export** button allows exporting samples results data to a .csv file for further treatment. Users may choose to export the **Summary** of the analyzed samples which includes the information displayed in the sample table, **Details** of the analyzed sample run which include the detector counts over time used to create the graphs, or both.

Users may also **Print** the samples results. When clicking on the print button, a separate window opens giving users access to a print preview and the options to change background color, put a watermark, export the results in pdf form and e-mail the results.

Section 5.7.4 – Sample Settings

Samples parameters are located in the **Sample Settings** section. To perform an analysis, users must first add samples to the group by clicking the “**+ Sample**” button. Upon clicking the “+ Sample” button, users will be prompted to specify the following information: **Number of samples** to be analyzed, **Tray** where samples are located, number of **Runs per Samples**, **Density** of samples, **Dilution Factor** and the **Method** to be used for the analysis. Users may leave blank the fields marked with an asterisk * if parameters are not common to every sample. If using an External Injection Module, the Tray field does not need to be filled. *Note that only methods with an associated calibration may be used to analyze a sample.*

The **Dilution Factor** allows the measurement of heavier samples that can otherwise not be sampled. The **Dilution/Dilution Factor** field corresponds to the quantity, in decimal value, of pure substance within the sample to be analyzed. For example, if a sample contains 20% of heavy gas oil and 80% of isooctane, the dilution value is “0.2”. For a 50%/50% mix, the dilution value would be “0.5”.

After specifying the information general to all samples, users must then enter the **Name** of each sample information in the corresponding table. If using an Autosampler, users will also need to specify **Tray** (if not common) and **Vial Number** corresponding to each sample. If using an External Injection Module, the tray and vial boxes are greyed out. Users may choose to **Include/Exclude** a sample from the analysis by checking/unchecking the textbox next to the sample number.

Users may import/export sample tables by using the “**Import**” and “**Export**” buttons. Exported and Imported tables are in .csv format and may be transferred from another analyzer or group to avoid having to repopulate sample tables.

Once all the information is entered in the Sample Settings section, the analysis is started by pressing the “**Run**” button. Users may track the progress of the analysis by monitoring the progress bar at the bottom right of the LUI. The LUI will also highlight the sample currently analyzed.

Section 6 – ATOM PAL LSI Autosampler

This section details information about the ATOM autosampler set up and use. For information about autosampler assembly, please contact ATOM Instrument. Once the Autosampler is completely assembled, it must be configured for the specific task of running analyses. The subsequent sections are meant to guide users through the initial setup procedures, and procedures to install and set up the necessary Autosampler modules, referred to as PALmodules. *Note, a glossary of definitions is located in Section 6.8 – Glossary of Definitions*.

Note that the setup order must be followed as listed in this manual as the order is dictated by the inter-dependency of modules. If a particular list item is already installed or set up, it may be skipped.

Section 6.1 – Autosampler First Start

If the Autosampler has been previously set up, when powered ON, the Input Terminal will boot up to the "Home screen" as shown in *Figure 45 with* all necessary PALmodules installed, follow the "Teaching" procedures explained in Section 6.7 – Modules Teaching to finish autosampler setup. If the PALmodules have not been installed, the Input Terminal will boot up to the "Home screen" shown in *Figure 46.*

Please note that even if the PALmodules have already been installed, they will need to be reconfigured using the "Teaching" procedures whenever the Autosampler is reassembled.

Figure 45 Home Screen with PALModules Installed

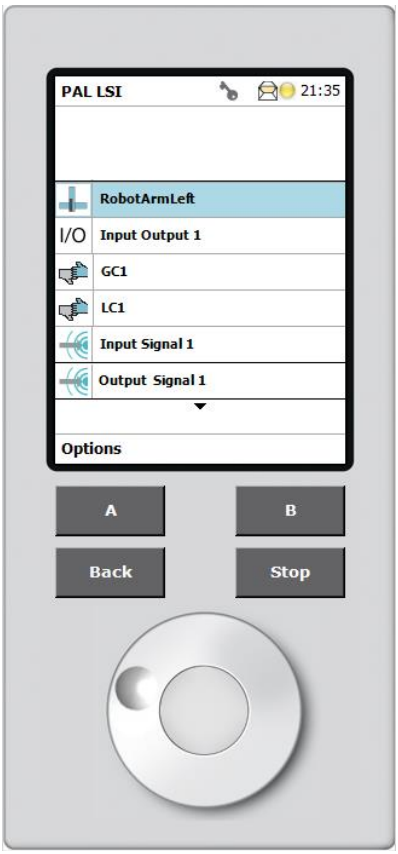


Figure 46 Home Screen with PALModules not Installed

Section 6.2 – Autosampler Home Screen

When powered ON, the Autosampler boots up to the "Home Screen" shown in *Figure 47*.

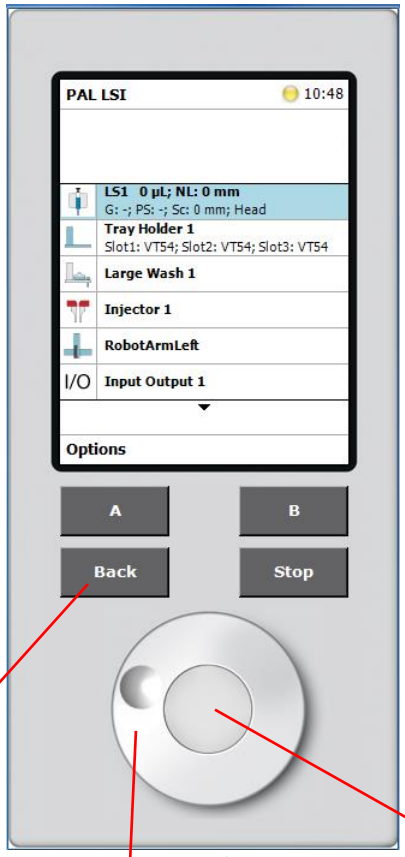


Figure 47 Autosampler Home Screen

*At any time the "**Back**" button is pressed, the Terminal will **exit** from the current menu to the previous one.*

*Once the desired menu item is highlighted, the **center button** may be pressed to **select** that menu option.*

*Turning the **knob wheel** clockwise or counter-clockwise allows users to **scroll up or down** menus and lists.*

Section 6.3 – Extended User Level

The ATOM autosampler possesses two user access levels: User and Extended User.

In order to modify any autosampler parameter, the “Extended User Level” must be selected to access the various setup menus. User access level may be change by pressing and holding both “A” and “B” buttons in the Home Screen to bring up the “Change Access” screen (*Figure 48*). Users may change access level by scrolling to the desired level. An asterisk * indicates the current user access level.

Please note that users must access the Extended User Level to perform any modifications to the autosampler, as the majority of menus are only accessible through the Extended User Level.

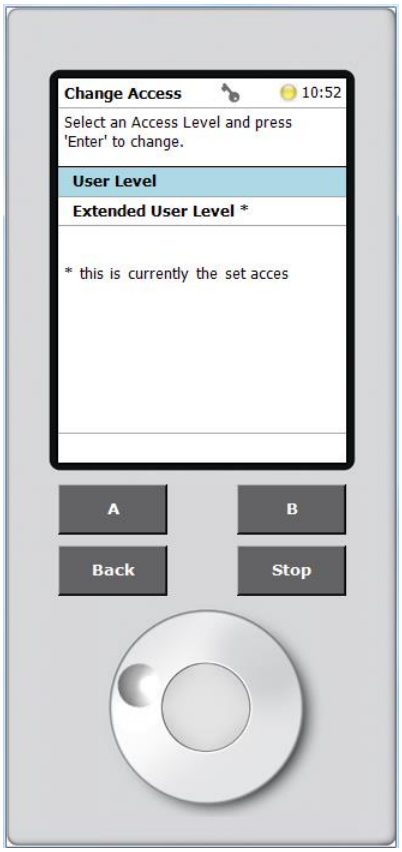


Figure 48 Extended User Level Access

Section 6.4 – Preliminary Setup

Th preliminary setup consist of the first step for Autosampler installation and include basic setup such as regional settings, time and date and naming of the autosampler.

Section 6.4.1 – Regional Settings

Regional settings allows the user to modify language and the region where they are located. To modify Regional settings, press “A” (Options) in the Home Screen to go into the Service menu. In the Service menu, select “Installation” (*Figure 49*).

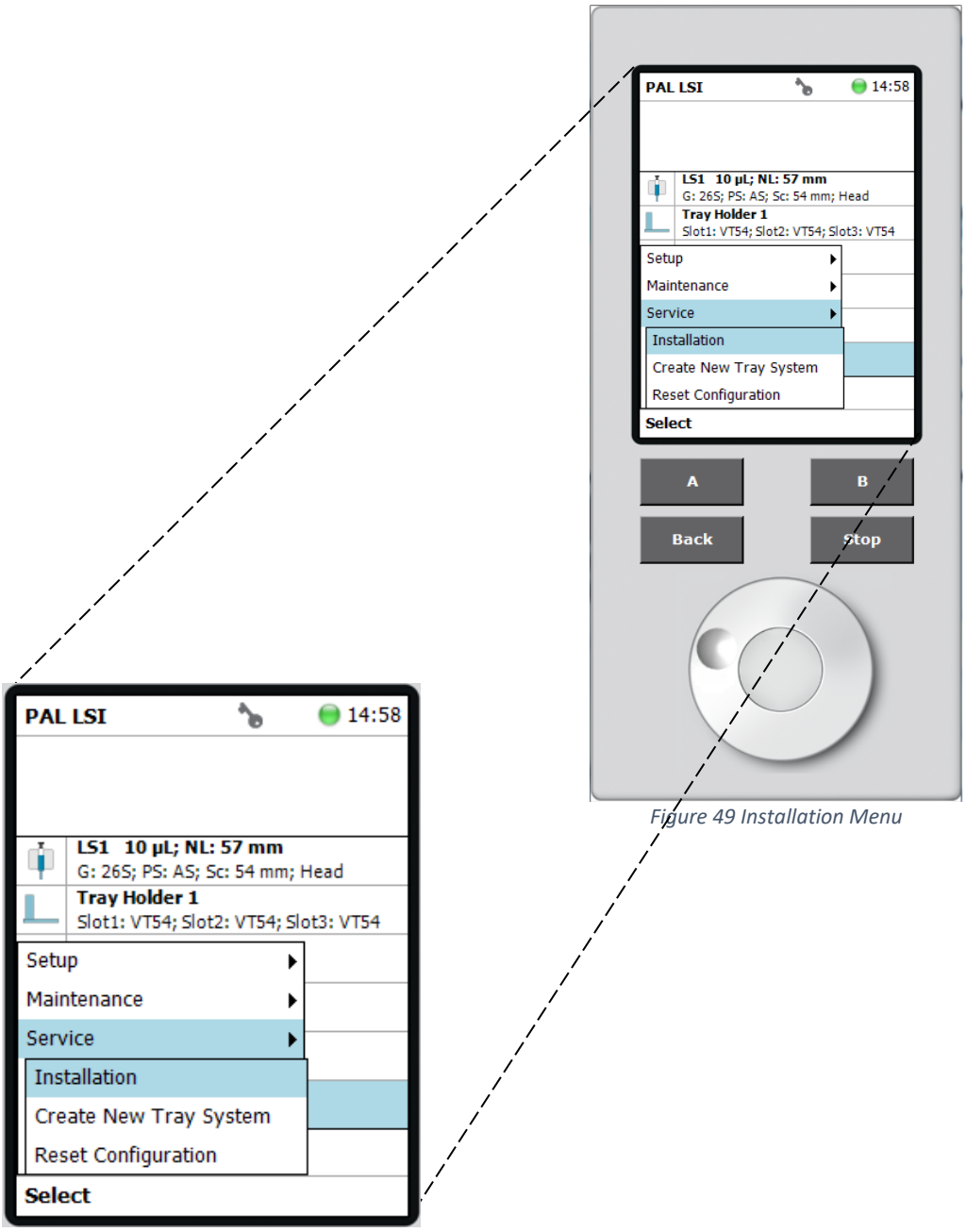


Figure 49 Installation Menu

In the “Installation” menu select “Set Regional settings” (*Figure 50*).

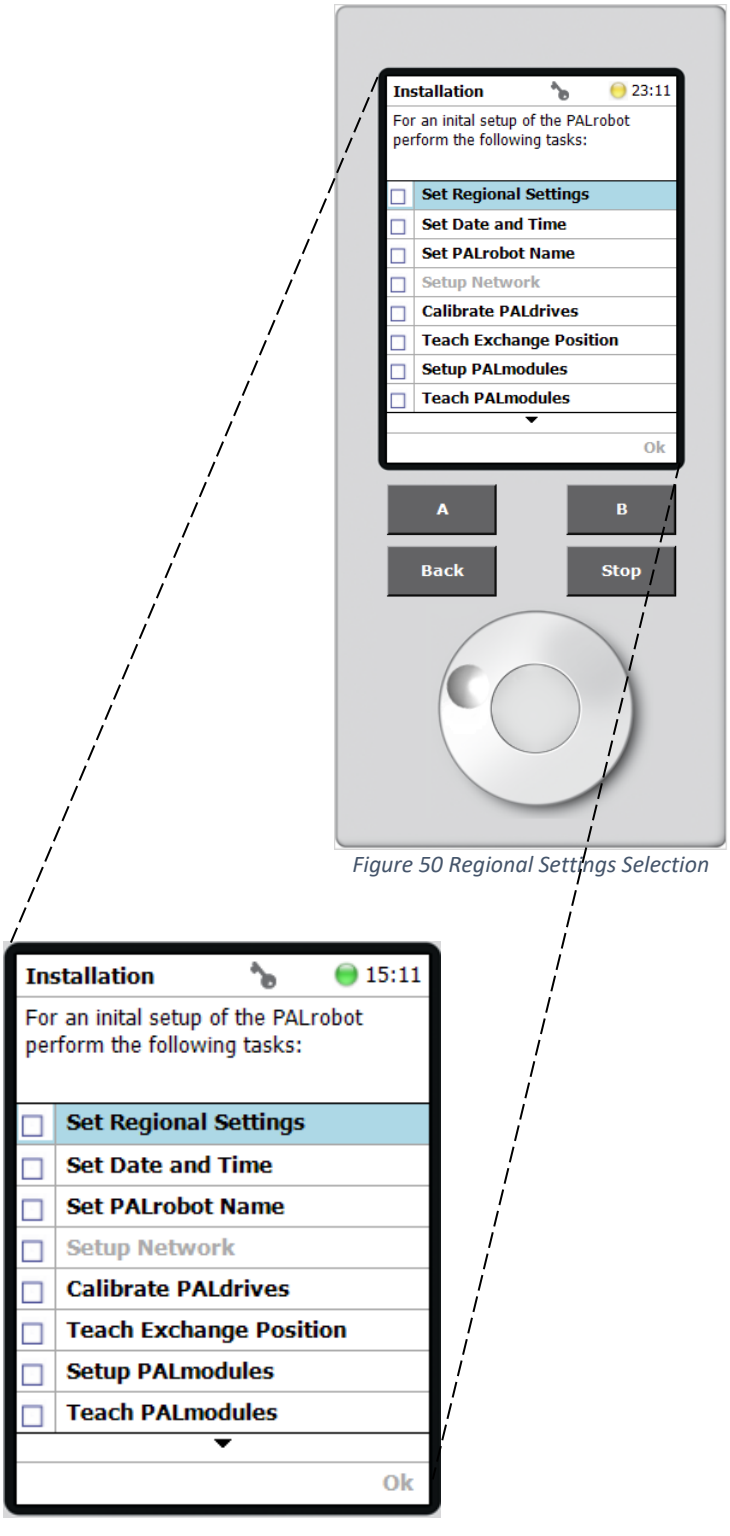


Figure 50 Regional Settings Selection

In the “Regional Settings” menu, select the desired Language setting, and Region setting (*Figure 51*). By default, those are set to English and United States. Press “B” (OK) to exit to the Regional Settings menu.

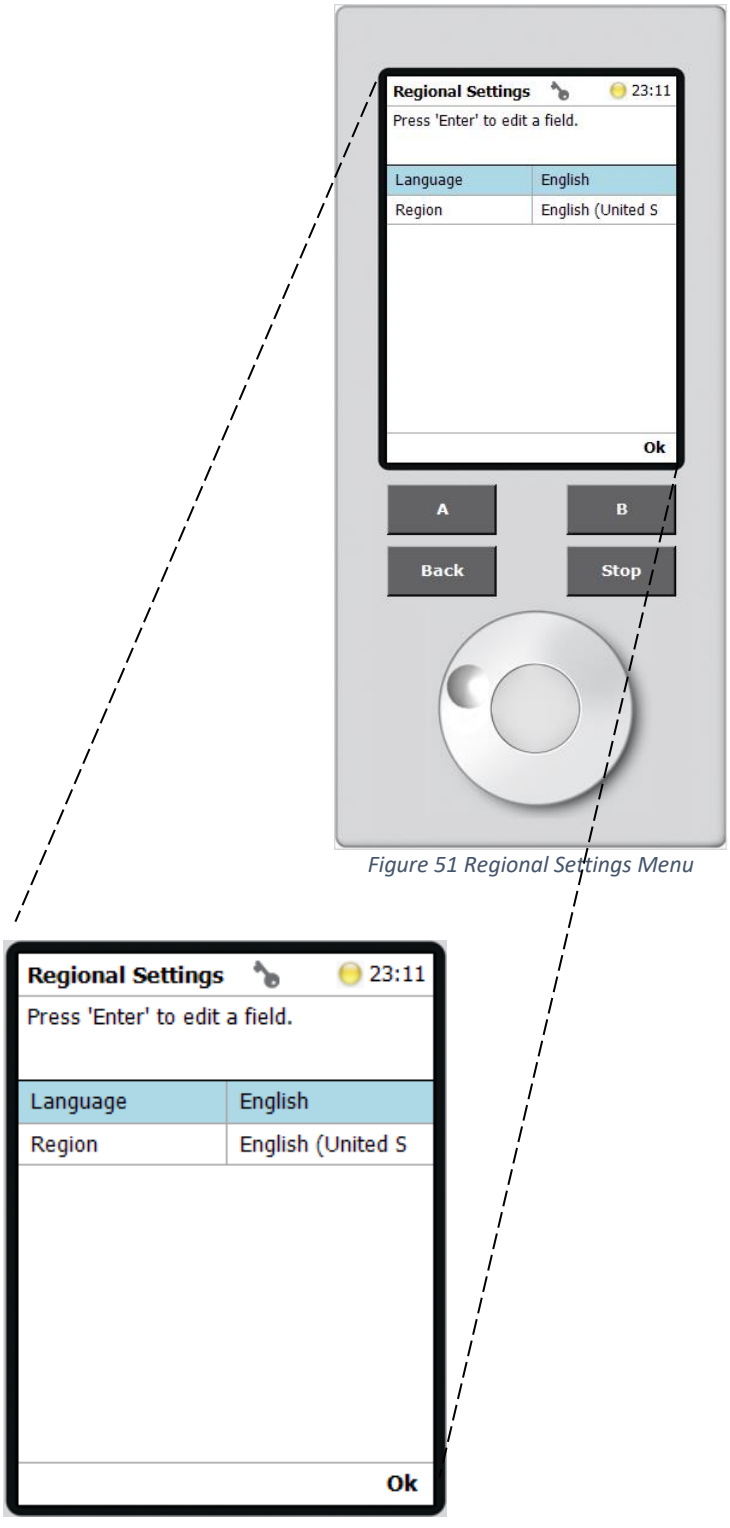


Figure 51 Regional Settings Menu

Section 6.4.2 – Time and Date Settings

The Time and Date settings allows users to modify the time and date of the autosampler. To modify Time and Date settings, press “A” (Options) in the Home Screen to go into the Service menu. In the Service menu, select “Installation” (*Figure 52*).

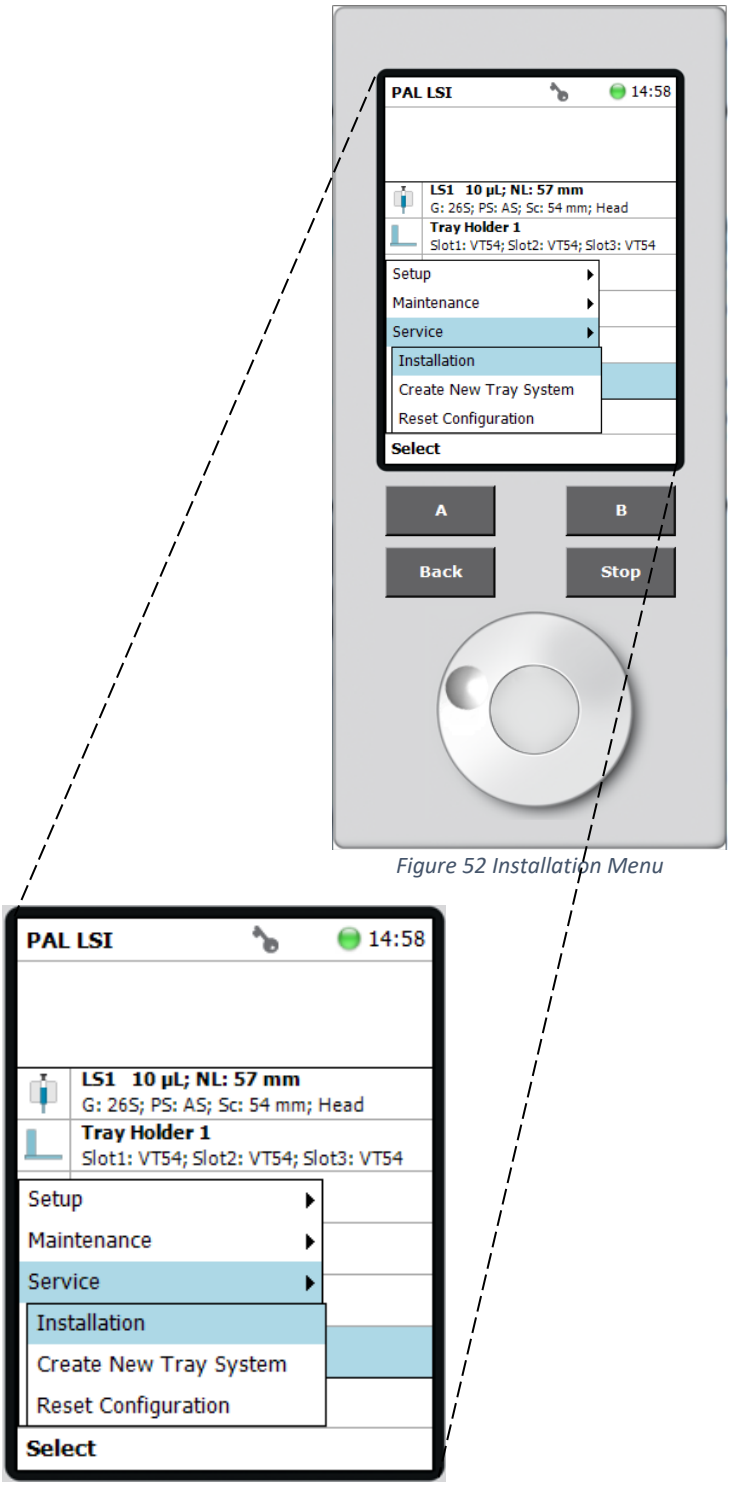


Figure 52 Installation Menu

In the “Installation” menu, select “Set Date and Time” (*Figure 53*).

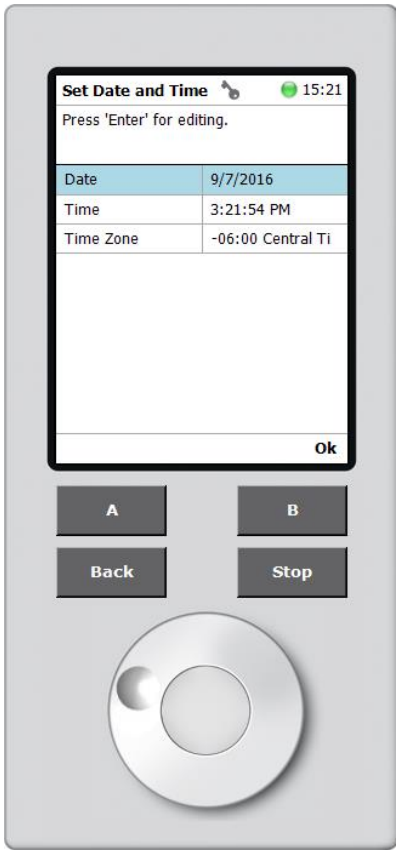


Figure 53 Date and Time Menu

Set the current date and time (24 hour format) as shown below and press “B” (OK) when finished.

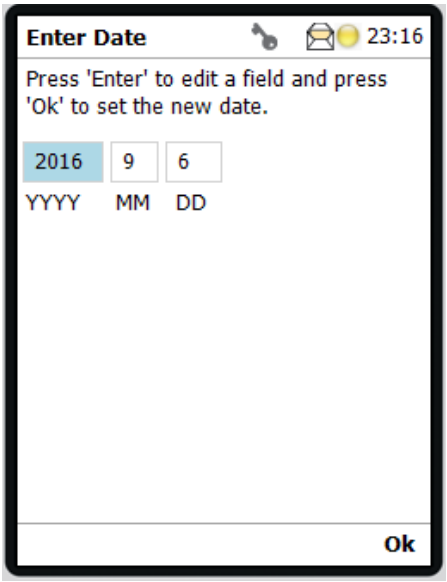


Figure 54 Date Settings

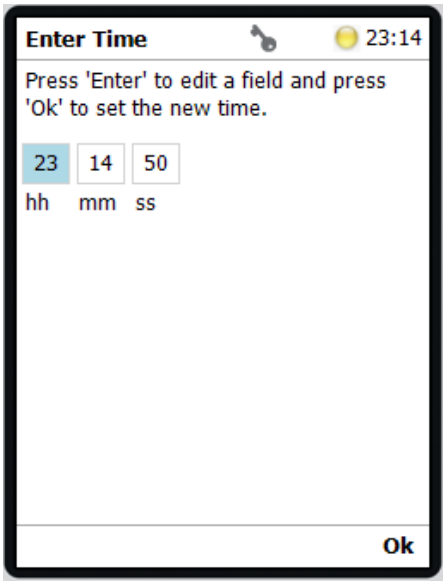


Figure 55 Time Settings

From the drop-down list, select the correct Time Zone (*Figure 56)*.

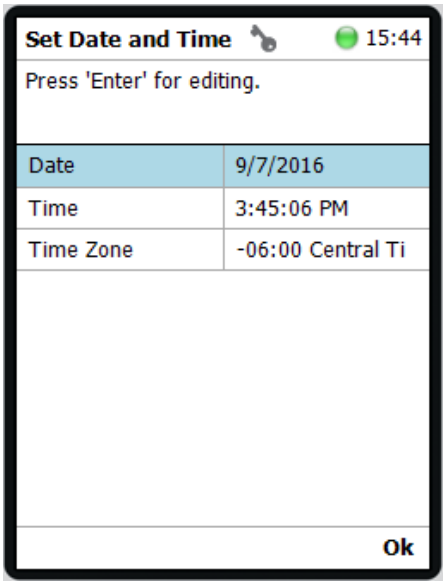


Figure 56 Time Zone Settings

Press “B” (OK) to exit back to the “Installation” menu.

Section 6.5 – Communications Setup

For the autosampler to communicate with the computer, both systems must be configured with matching information. The following section details how both the computer and the autosampler are configured to ensure proper communication.

Section 6.5.1 – Autosampler Network Setup

The Network settings allows users to modify network configuration of the autosampler. To modify Network settings, press “A” (Options) in the Home Screen to go into the Setup menu. In the Setup menu, select “Setup Network” (*Figure 57*).

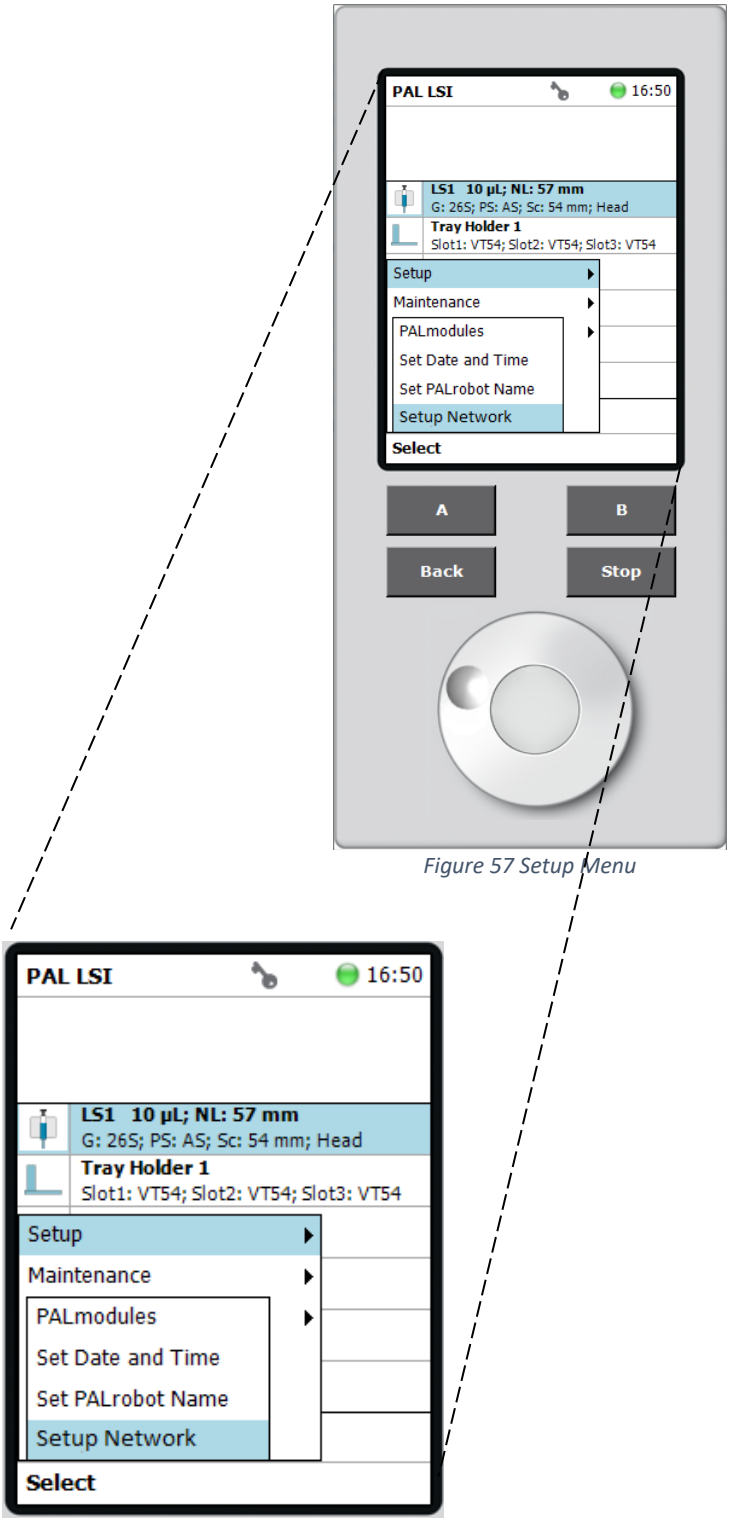


Figure 57 Setup Menu

In the Setup Network menu enter the appropriate IP Address, Subnet Mask, and Default Gateway. The MAC address is machine specific, and cannot be changed. Once all parameters are entered, press “B” (OK) to return to the Home Screen (*Figure 58*).

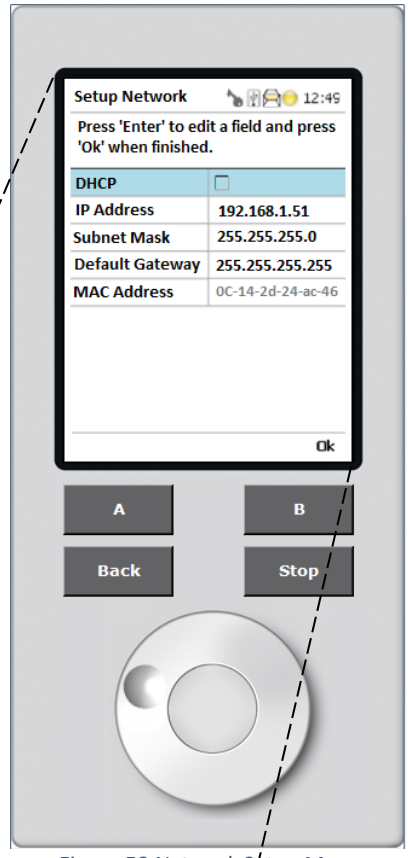
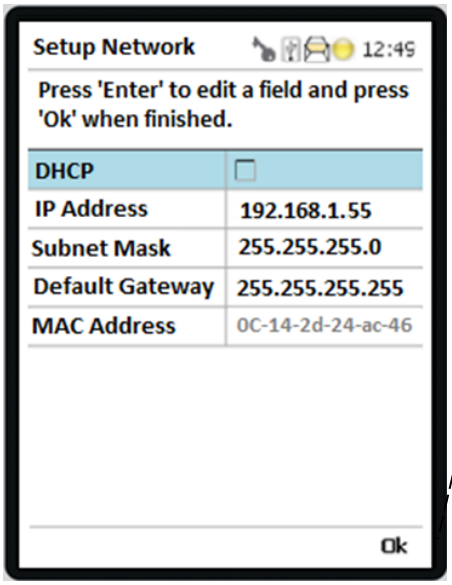


Figure 58 Network Setup Menu



Please contact IT department for Network information.

Section 6.5.2 – Autosampler-LUI IP address matching

Once the autosampler IP address has been set, it needs to be programmed in the ATOM LUI configuration file (LUI.exe.config) located at: **C:\ATOM\LUI\LUI.exe.config**. To modify, right click on the file and select "Open With" in the pop-up menu. Select "Notepad" from the list of available programs as shown in *Figure 59*.

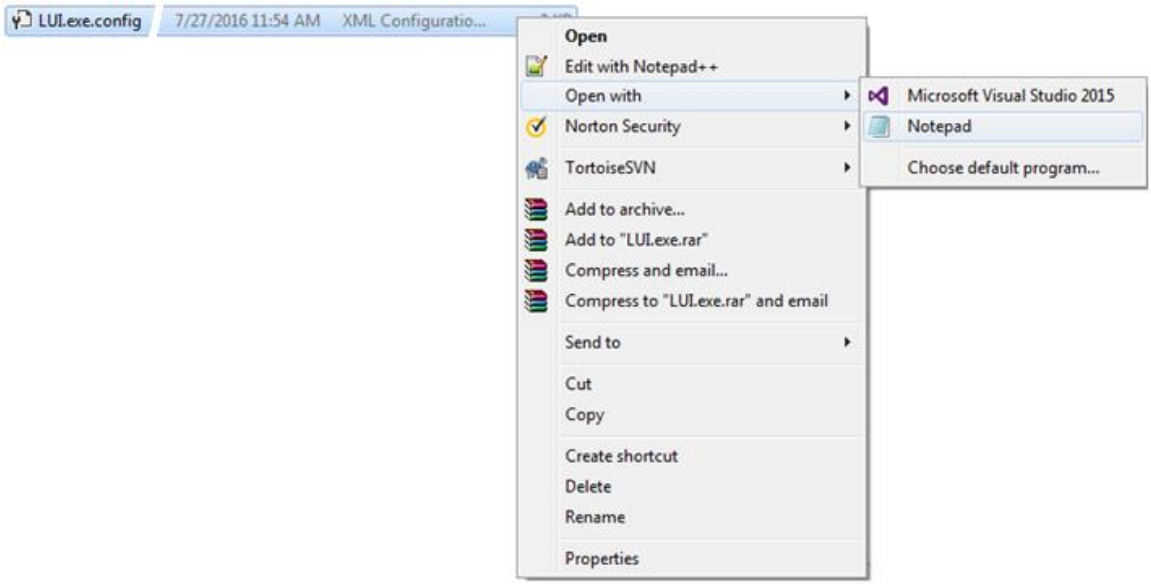


Figure 59 Opening the LUI Configuration File with Notepad

Once the configuration file is opened in Notepad, locate the setting "PALIP" value as shown in *Figure 60*. Modify the PALIP value to match the IP address set on the Autosampler as described in Section 6.5.1 – Autosampler Network Setup above. (*Figure 58*).

Please note that the IP address entered in the ATOM LUI config file must match the IP address entered in the autosampler Network Setup for the LUI to be able to communicate with the autosampler.

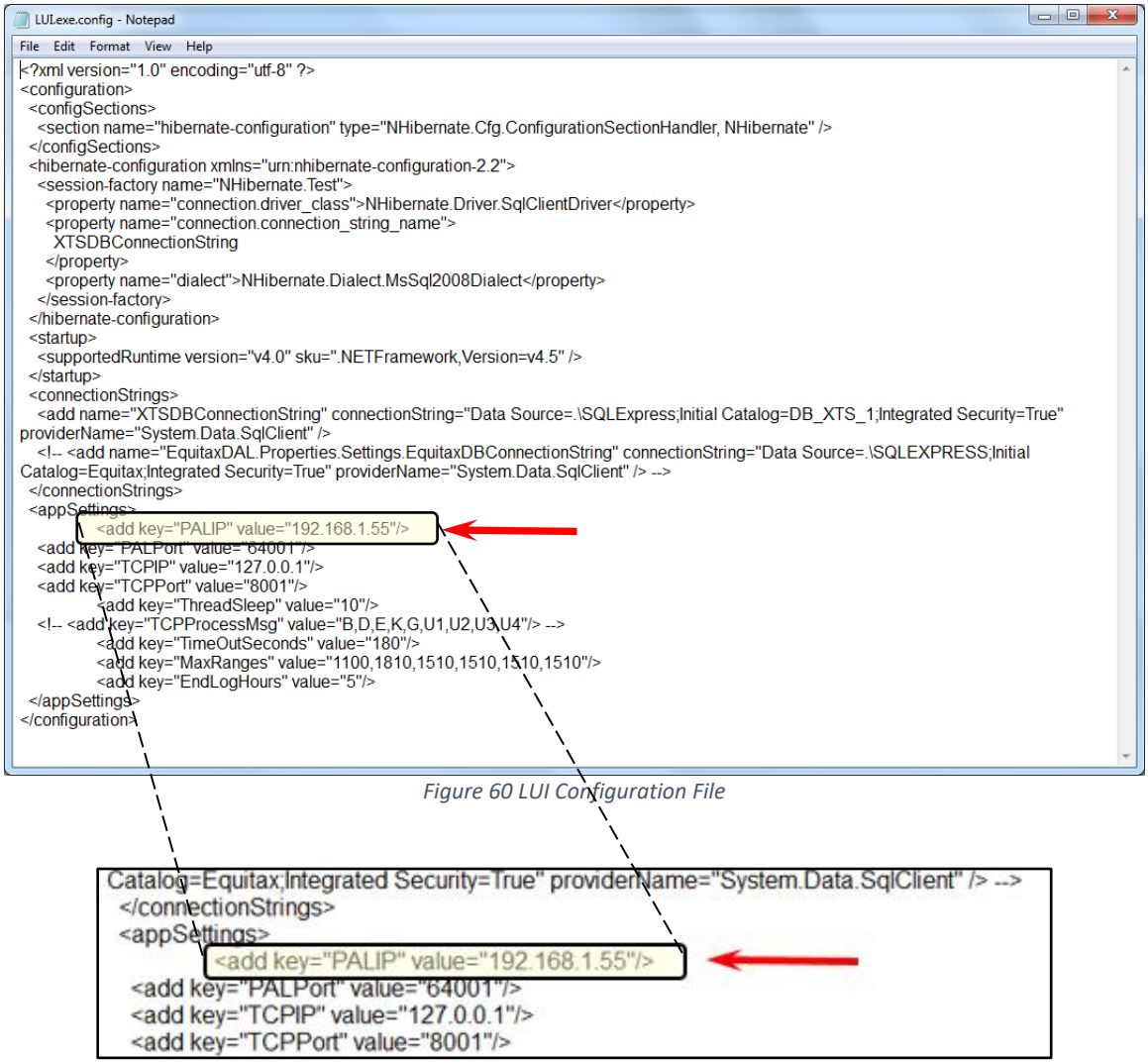


Figure 60 LUI Configuration File

Once the IP address has been modified to match the autosampler IP address, save the changes to the file and exit (*Figure 61*).

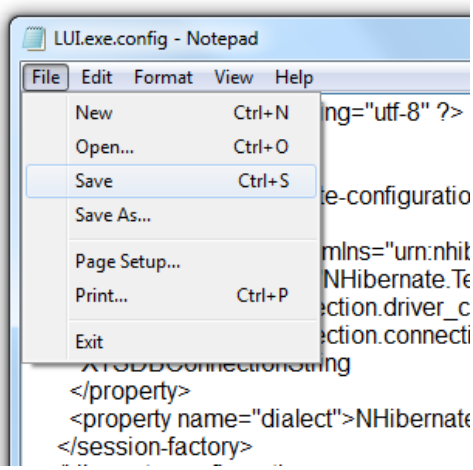


Figure 61 Saving the ATOM LUI Config File

Section 6.6 – PALModules Setup

This section details how each PALModule is installed and configured for use with the XT Series Analyzer.

Section 6.6.1 – PALdrives Calibration

The PALdrives calibration is an internal hardware calibration performed by the Autosampler. To calibrate PALdrives, press “A” (Options) in the Home Screen to go into the Service menu. In the Service menu, select “Installation”. In the Installation menu, select “Calibrate PALdrives” and press “B” (Calibrate) which will start the automatic calibration process (*Figure 62*).

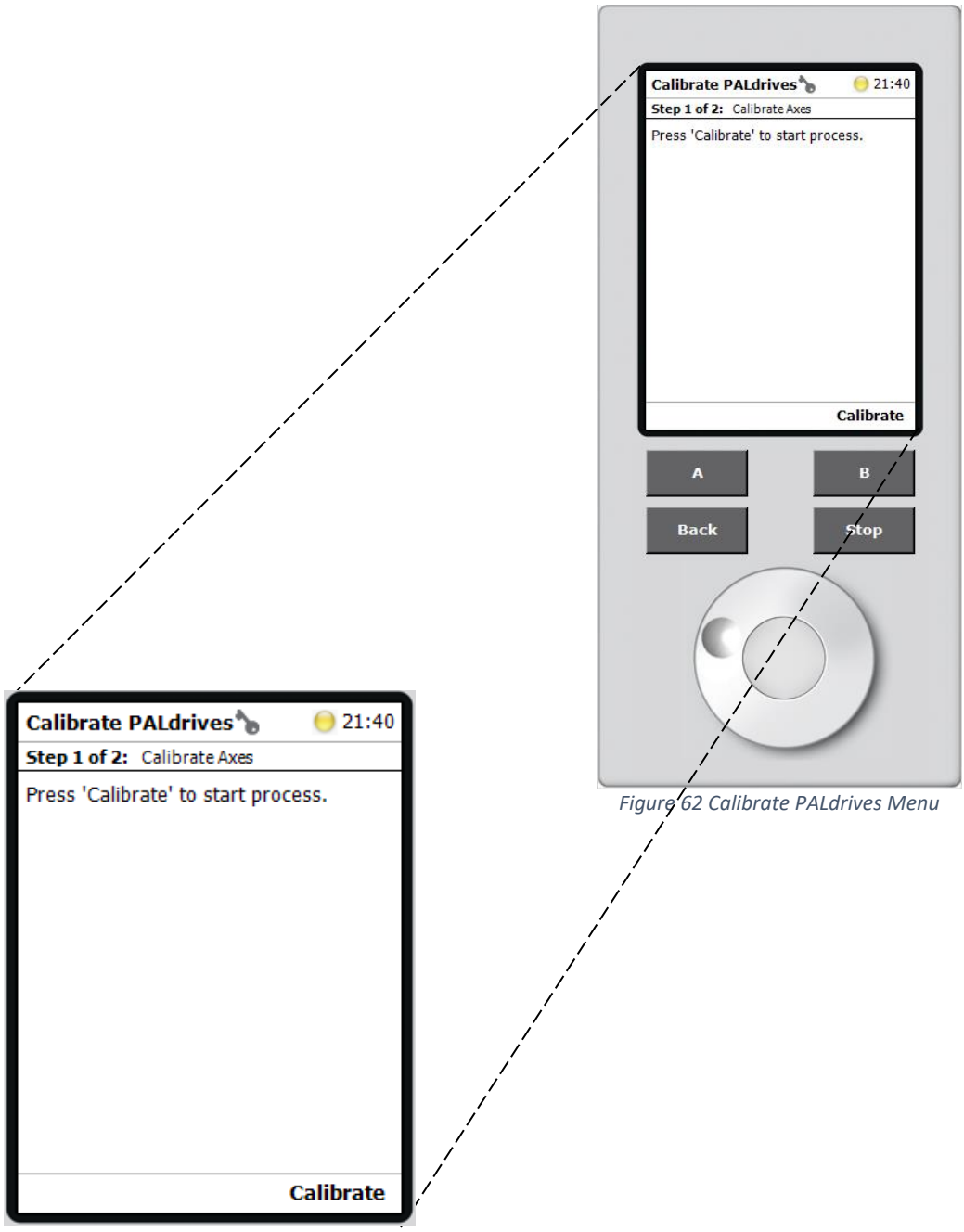


Figure 62 Calibrate PALdrives Menu

When prompted by the Autosampler, after completion of the calibration procedure, press “B” (OK) to exit to the “Installation” screen. The PALhead will return to the “Home” position. (*Figure 63*)

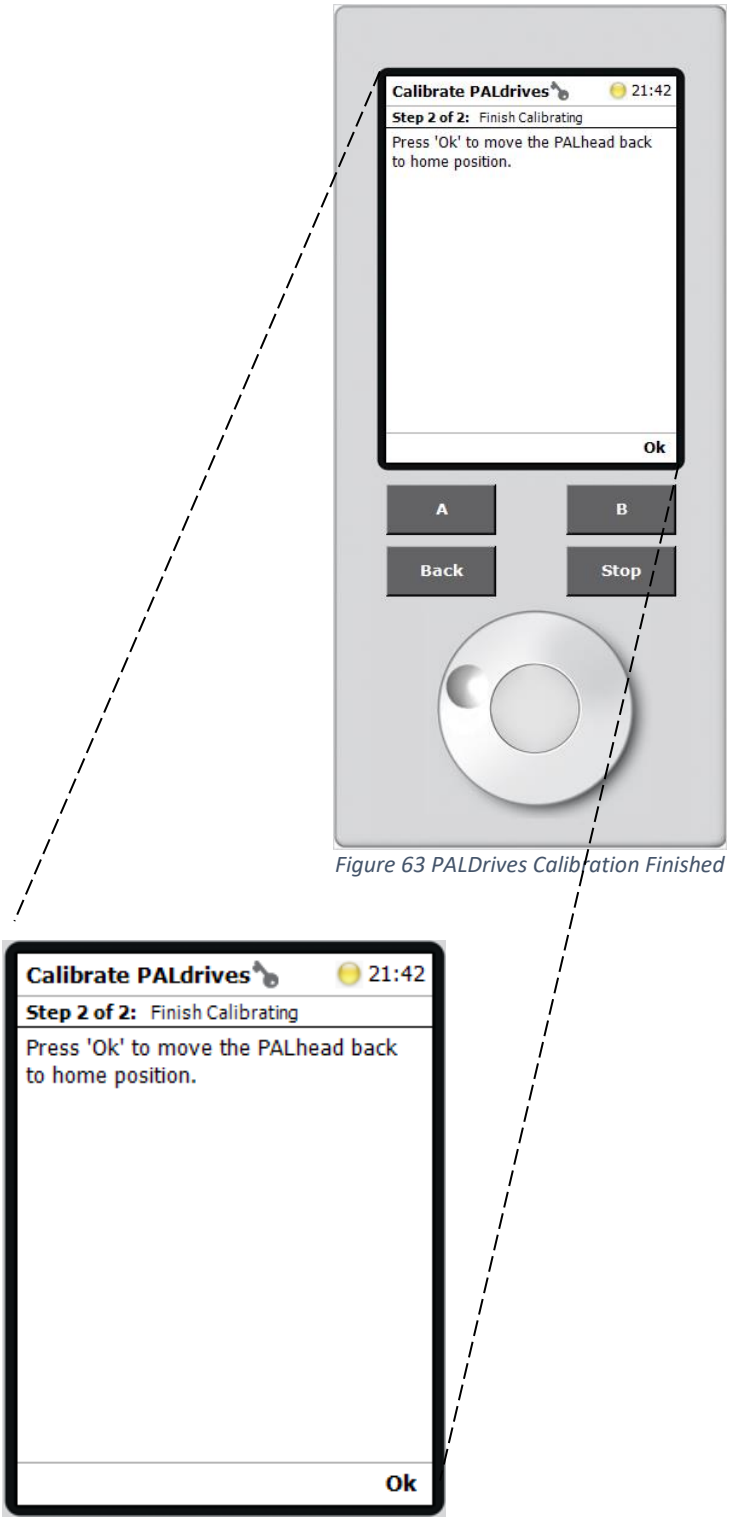


Figure 63 PALDrives Calibration Finished

Section 6.6.2 – Exchange position

When a syringe has to be installed or exchanged, the PALhead moves to a preset position such that the syringe is easily accessible. This position is as termed the “Exchange Position”, and is user-programmed as explained in this procedure. To teach the Exchange Postion, press “A” (Options) in the Home Screen to go into the Service menu. In the Service menu, select “Installation”. In the “Installation” menu, select “Teach Exchange Position”, and when prompted, physically move the PALhead to the desired position (Figure 64). When finished, press “B” (Save) to confirm and exit to the “Installation” screen.

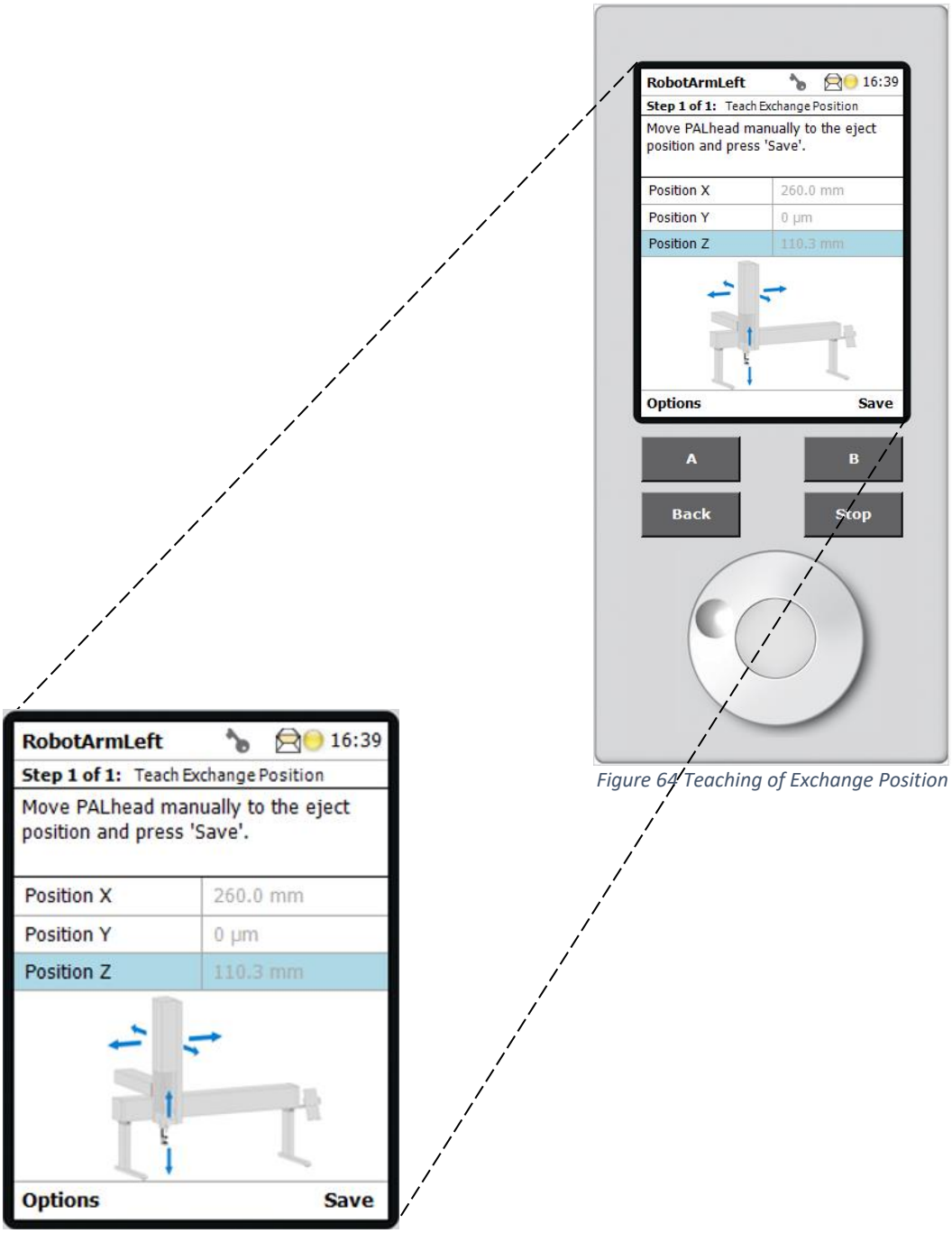


Figure 64 Teaching of Exchange Position

Section 6.6.3 – Programming of an ATOM-Specific Syringe

The XT Series Analyzer uses a non-standard syringe based on the default SYH207807 (LS D7mm; NL57mm) listed in the PALmodules. The default needle penetration depth (Max Pen Depth) specified for this syringe is 45mm, however, the XT Series Analyzer requires the needle penetration depth to be at 48mm.

Since the Autosampler does not allow any changes to be made to preset PALmodule parameters (syringe, in this case), an ATOM-specific syringe has to be defined with a specific needle penetration depth of 48mm.

The following procedure explains the steps to copy an existing syringe, modify the settings, and save the new syringe with desired parameters.

Section 6.6.3.1 – Creation of ATOM-Specific Syringe

To program a new syringe, press “A” (Options) in the Home Screen to go into the Setup menu. In the Setup menu, select “PALmodules” (*Figure 65*).

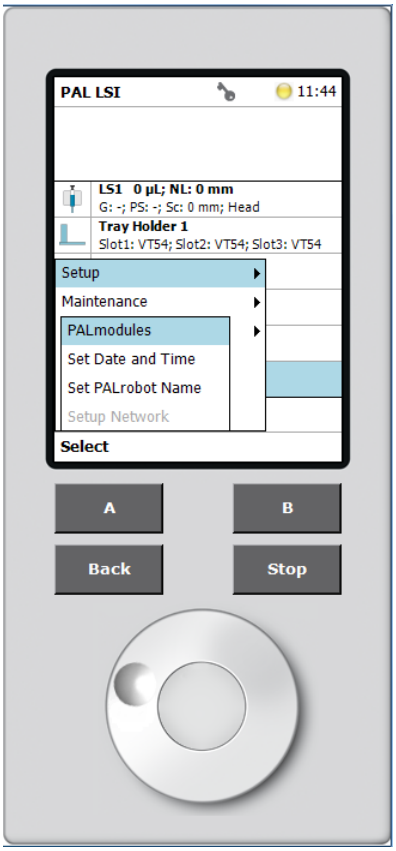


Figure 65 Setup Menu

In the PALmodules menu (*Figure 66*), select “Syringe Types” to open the list of available pre-defined syringes.

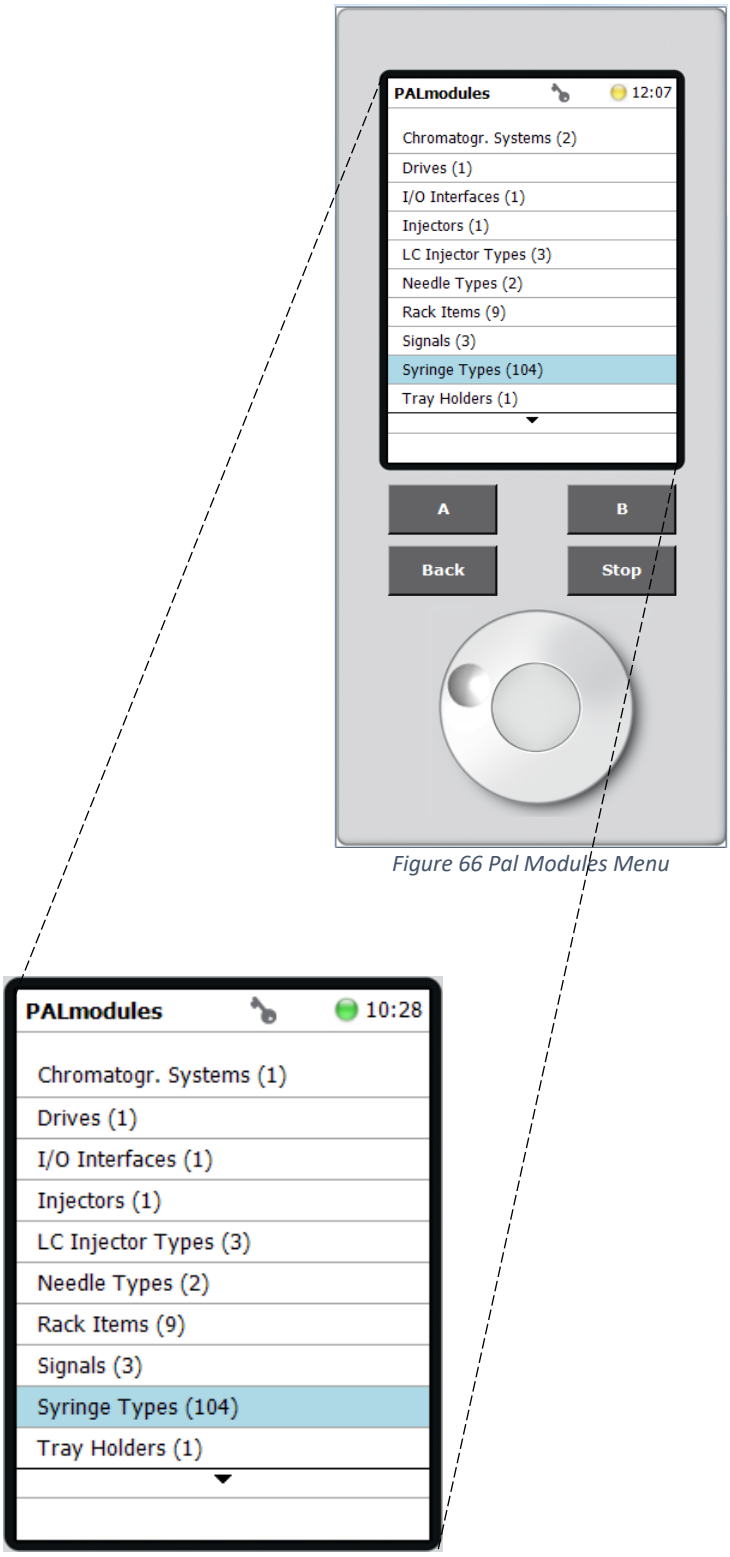


Figure 66 Pal Modules Menu

Scroll down the list to highlight the syringe SYH207807 (LS D7mm; NL57mm) (*Figure 67*).

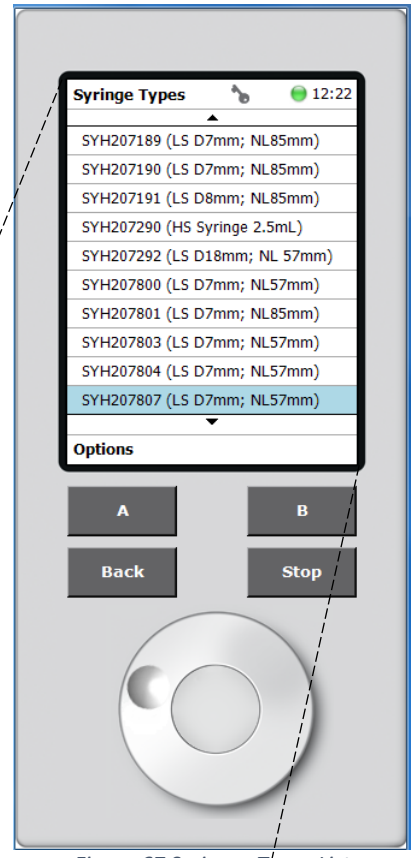
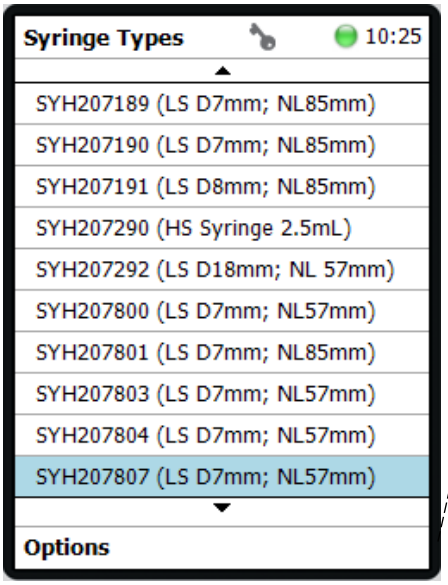


Figure 67 Syringes Types List



With the syringe SYH207807 highlighted, press “A” (Options), then “Copy SYH207807” (*Figure 68*).

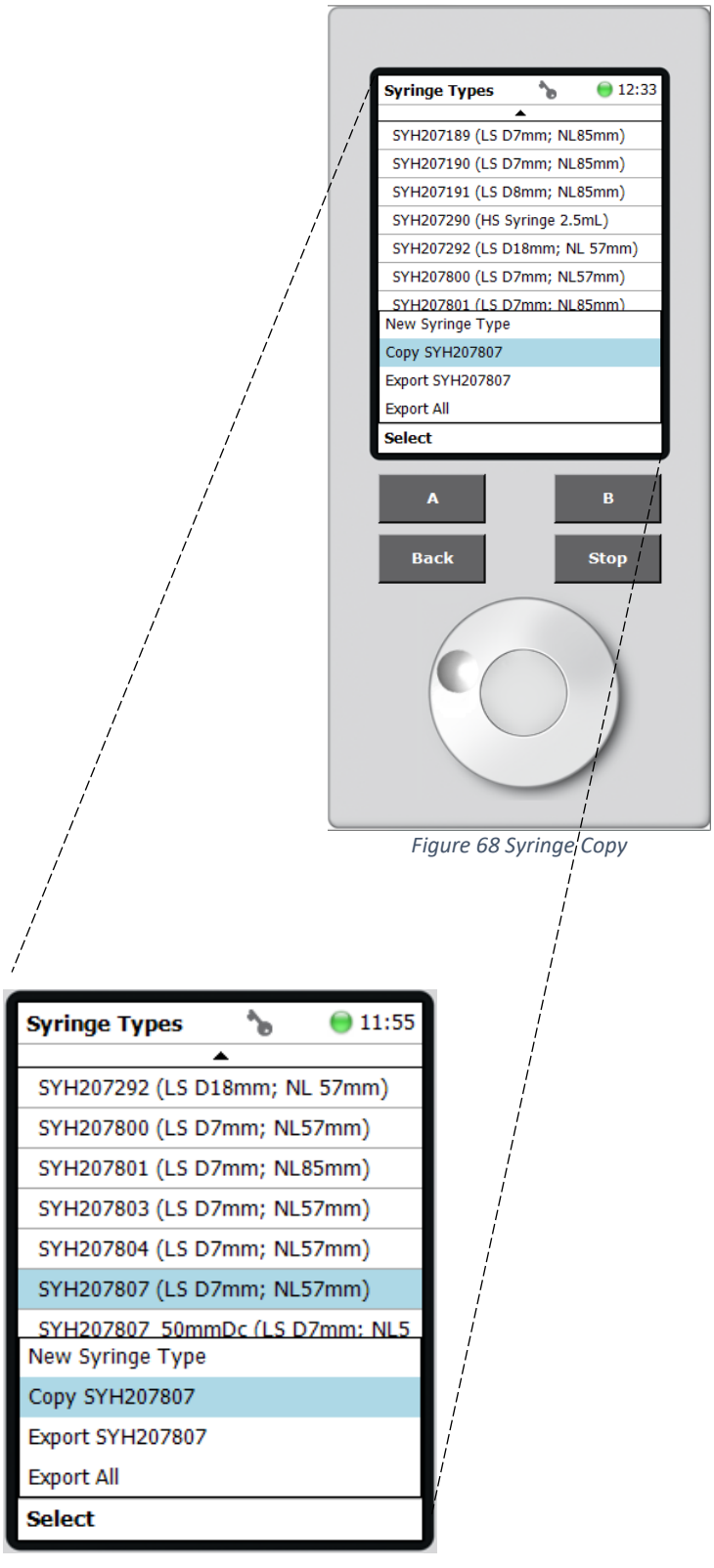


Figure 68 Syringe Copy

On the following screen, when prompted, enter the name “SYH207807_48mmD” (*Figure 69*) and press “B” (Copy).

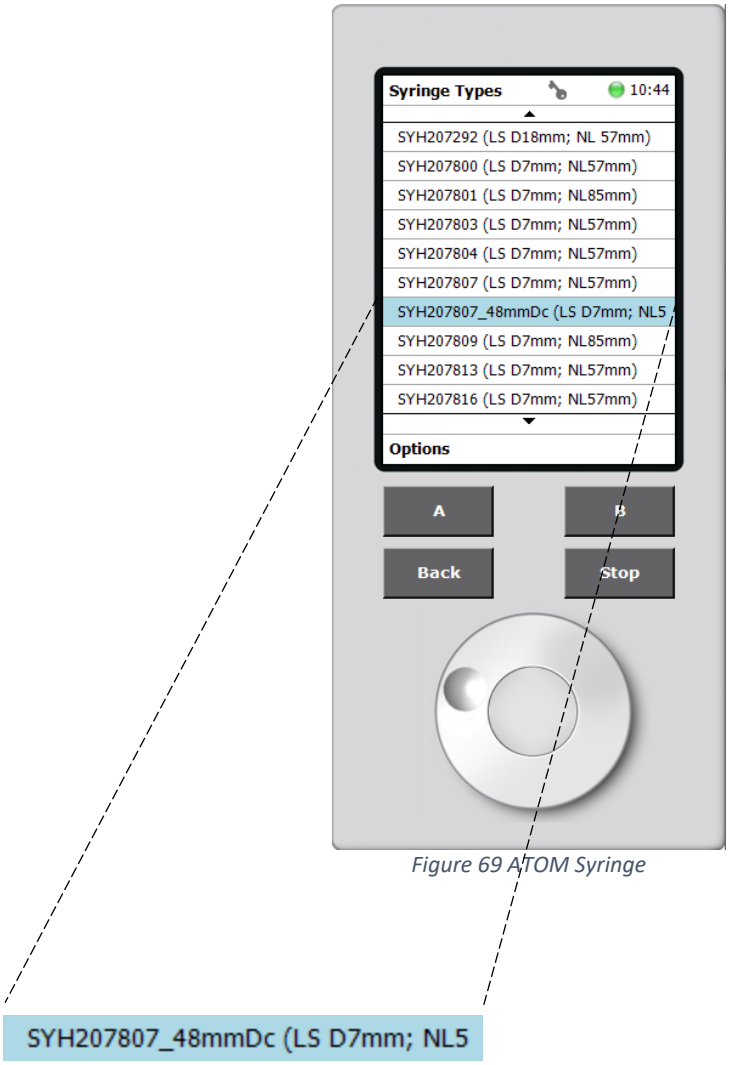


Figure 69 ATOM Syringe

Once the syringe is copied, the terminal returns to the list of all available syringes, including the newly created syringe.

Scroll up/down the list and select the syringe created. In the syringe parameters screen, scroll down the list and select “Max Pen Depth” (maximum needle penetration depth). Turn the knob clockwise to increase the maximum needle penetration depth to 48mm, and press the center button to confirm the new setting (*Figure 70*). Press the “Back” button until returning to the Home Screen.

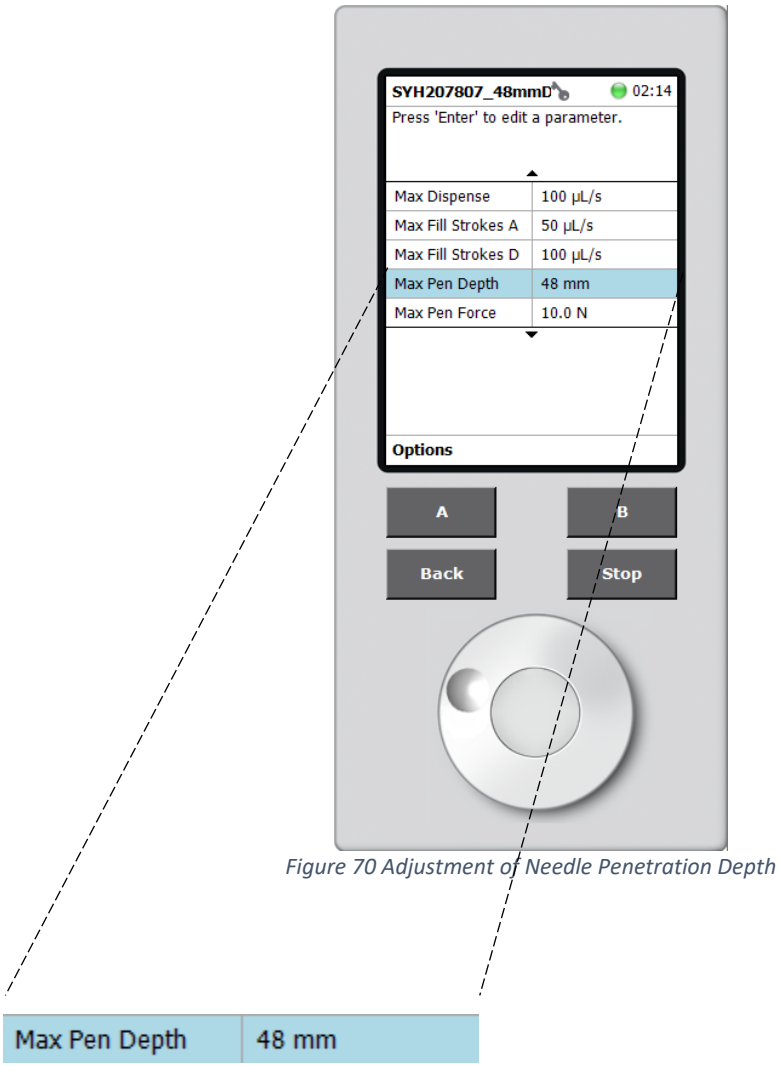


Figure 70 Adjustment of Needle Penetration Depth

Section 6.6.3.2 –Inputting of ATOM-Specific Syringe

To input the newly created syringe, scroll down and select “RobotArmLeft” (*Figure 71*).

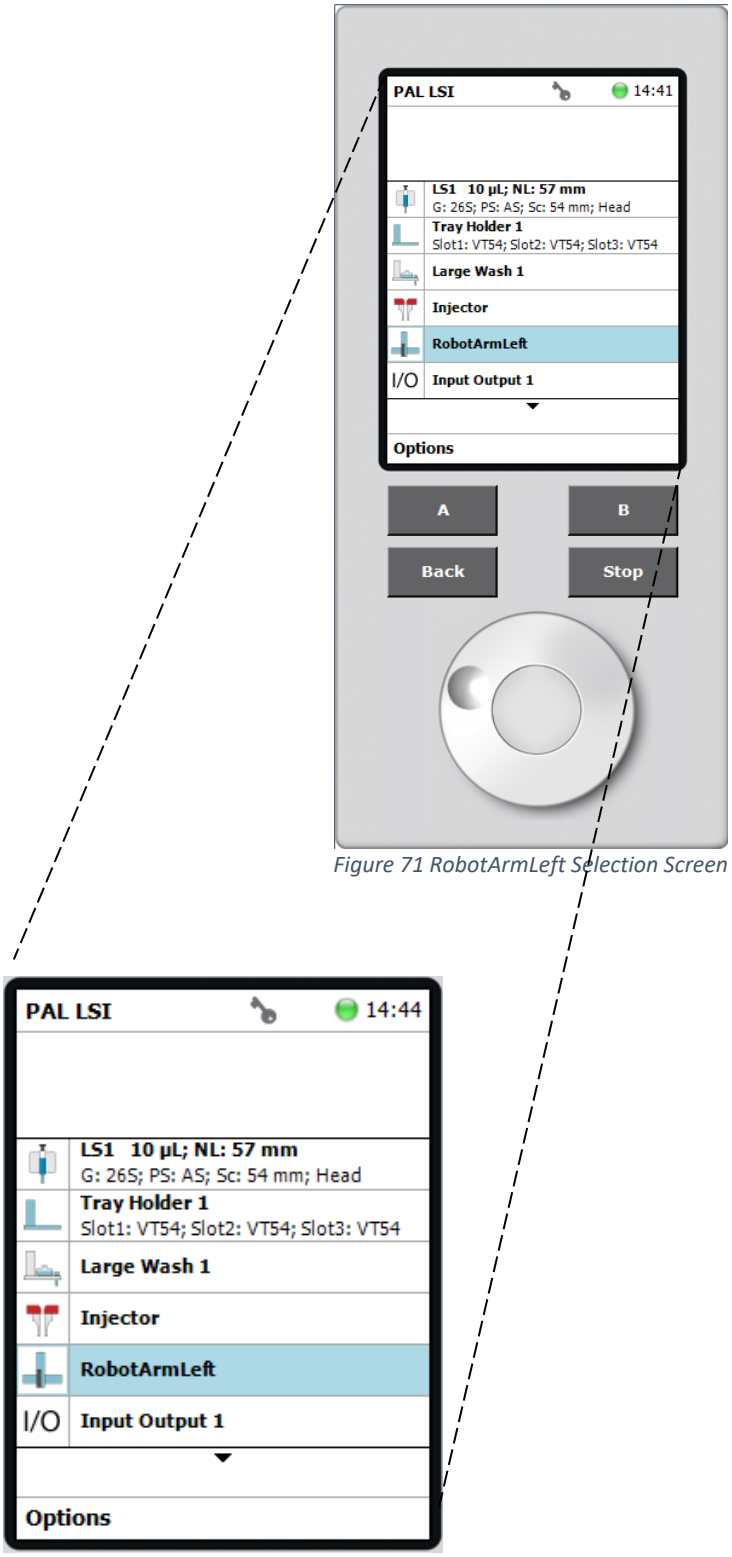


Figure 71 RobotArmLeft Selection Screen

Select “Adapter Control 1” to open a blank screen indicating that the PAL LS1 Tool has not been installed. Press the “A” (Options) button to add a new Adapter Control. When prompted, select the “D7/57” control type. Press the “Back” button and the screen to revert to the “RobotArmLeft” menu shown below in *Figure 72*.

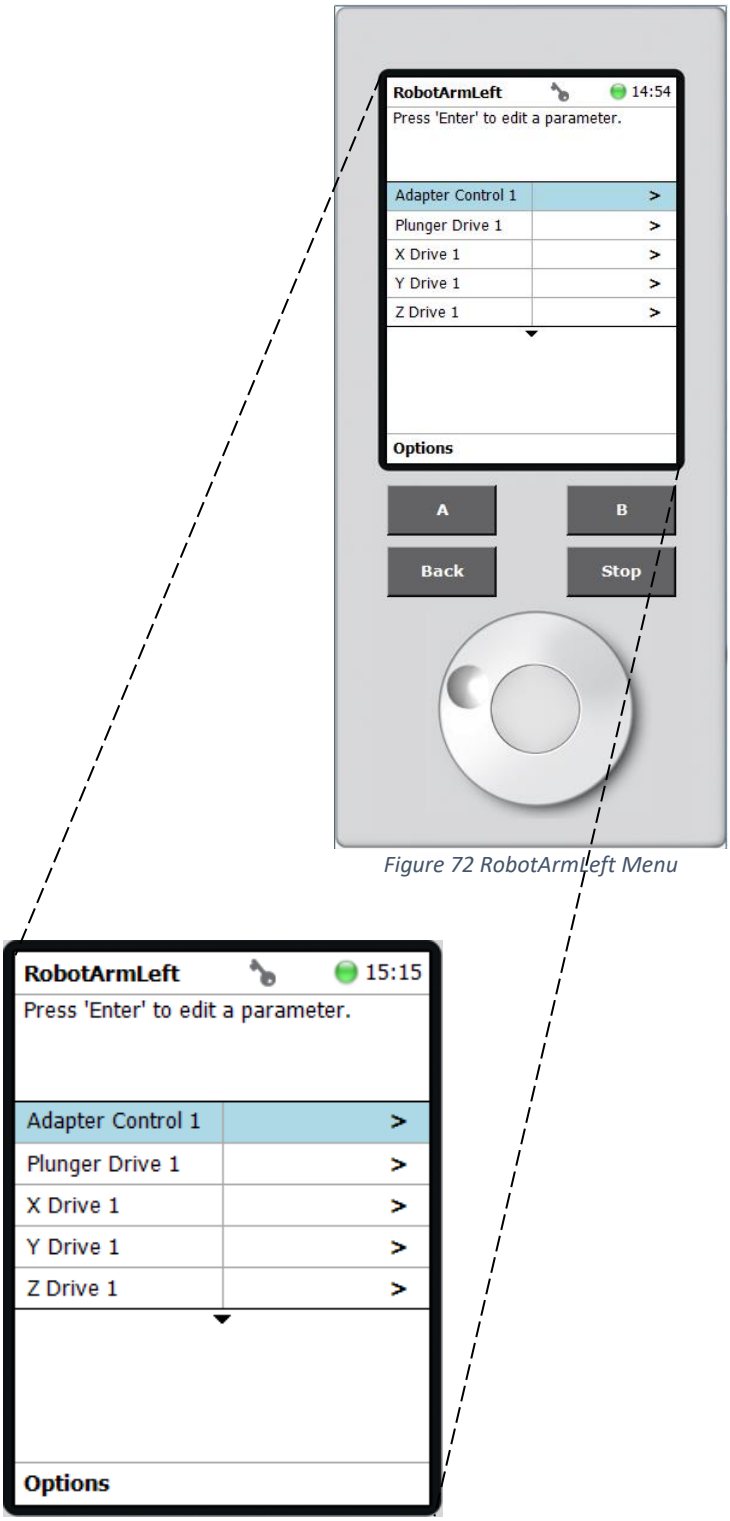


Figure 72 RobotArmLeft Menu

In the RobotArmLeft select “Adapter Control 1” again to display the newly added “LS1” tool as shown below in *Figure 73*.

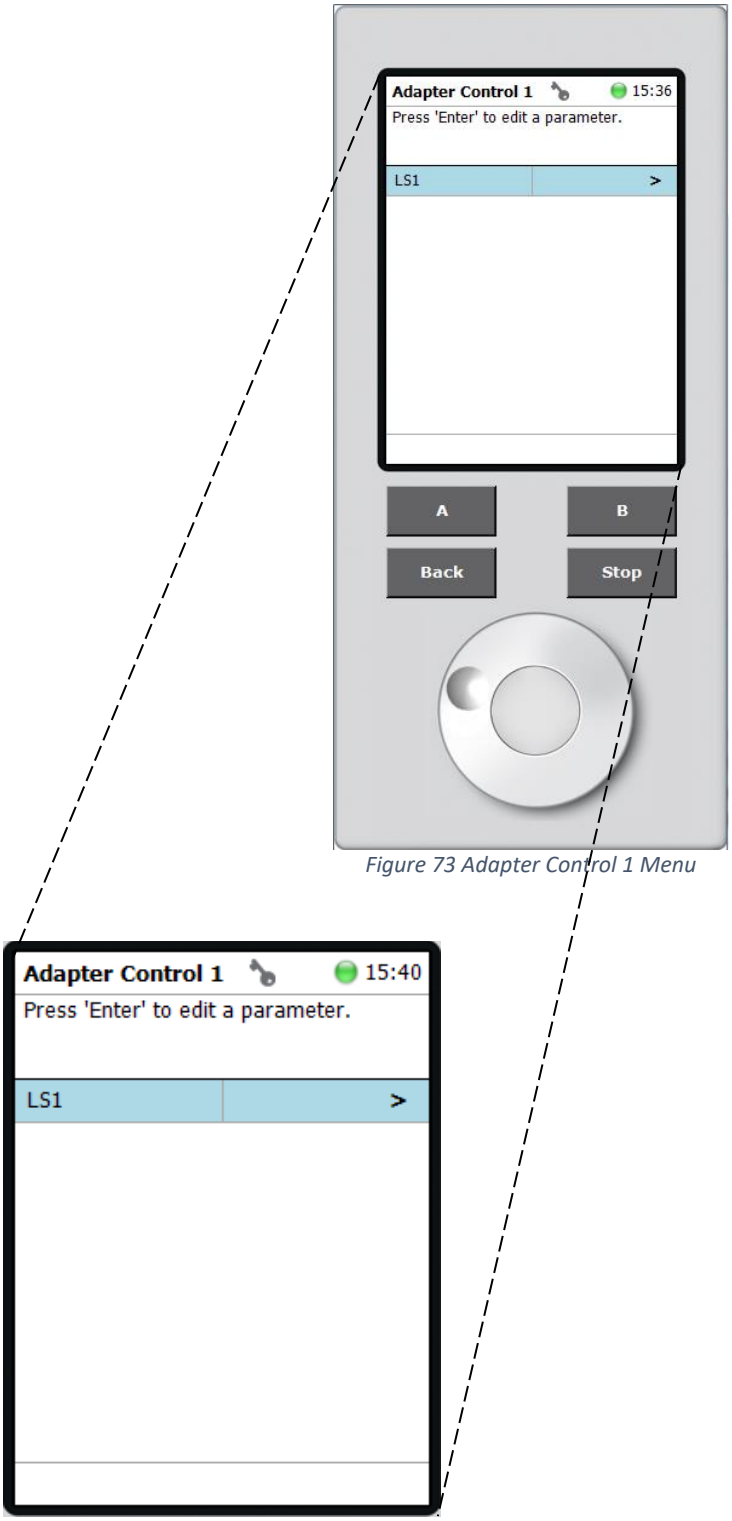


Figure 73 Adapter Control 1 Menu

Select “LS1” to access the LS1 options. In the options list, modify “Ndl Guide Type” to “NonMagn2mL” (*Figure 74*) and “Syringe Type” to the Atom-specific syringe programmed earlier (SYH207807_48Dc) (*Figure 75*). Then keep pressing “Back” until you exit out to the Home Screen.

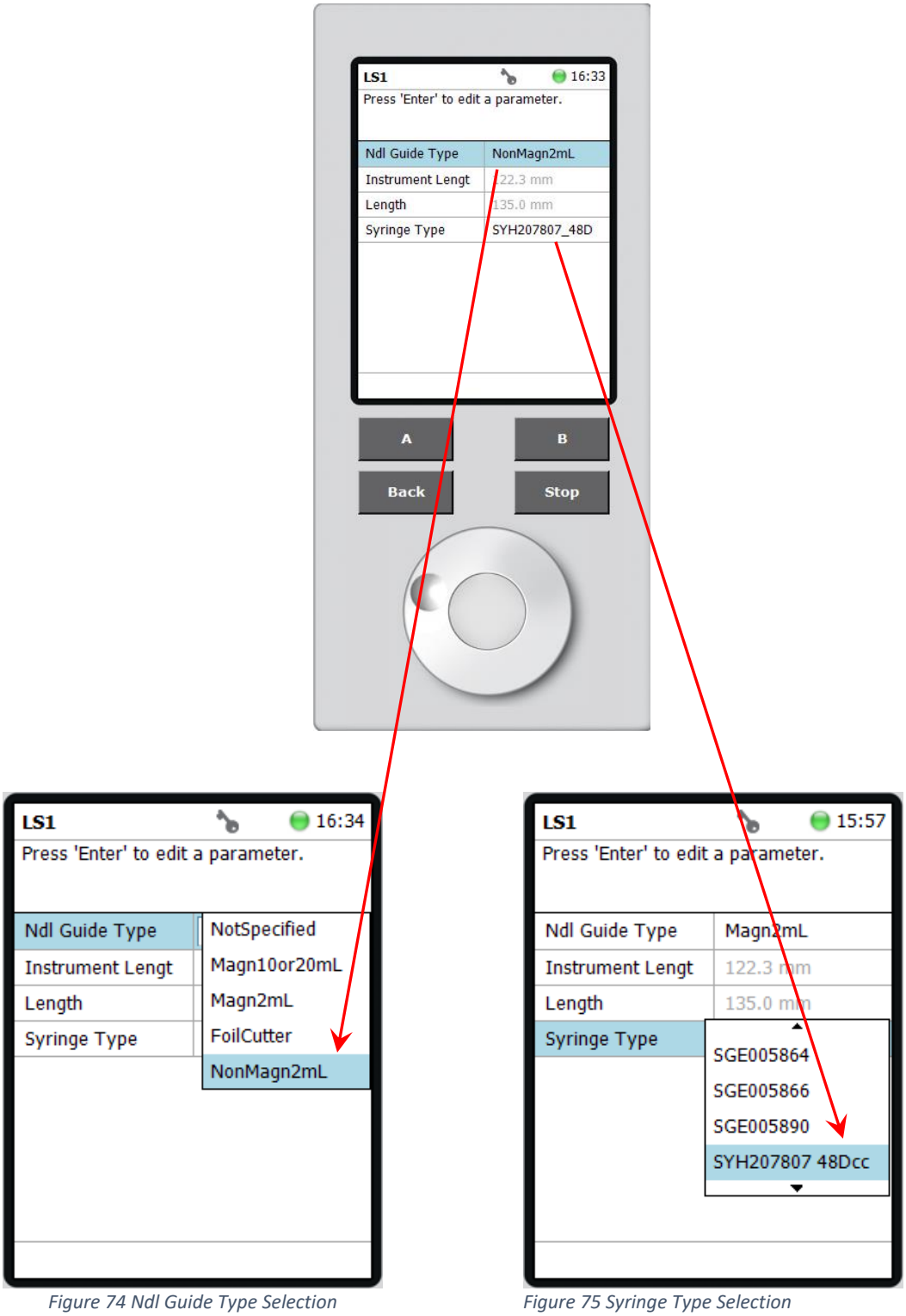


Figure 74 Ndl Guide Type Selection

Figure 75 Syringe Type Selection

Section 6.6.4 – Input Signal “SoftIn” Programming

The input signal “SoftIn” is the software interface between the ATOM programs and the Autosampler. It has to be defined in the Autosampler as the “channel” over which ATOM programs will communicate with it.

Two Autosampler locations need programing for the SoftIn to work:

- PALmodules -> Signals
- PALmodules -> Chromatograph Systems -> GC1 (GC)

Section 6.6.4.1 – Creation of SoftIn

From the Home Screen, press “A” (Options) then “Setup” and “PALmodules” (*Figure 76*).

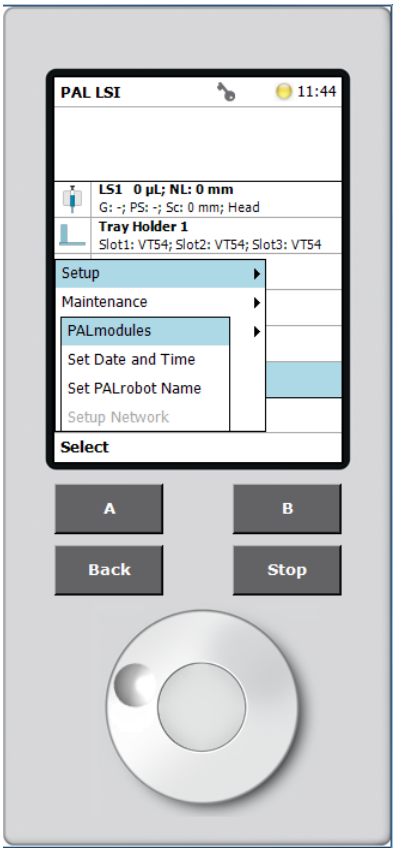


Figure 76 PALmodules Access Path

In the PALmodules menu, scroll down to select “Signals” and display all available default signals (*Figure 77*).

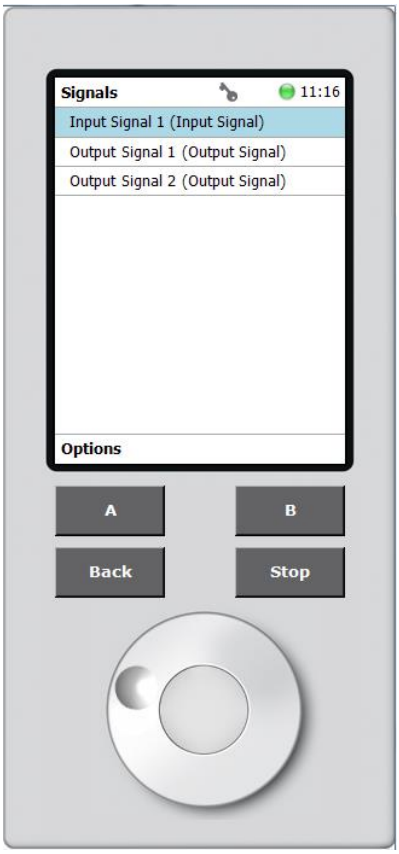


Figure 77 Signals Menu

Press “A” (Options) and select “New Signal” (*Figure 78*). In the following menu, select “Input Signal” as signal type (*Figure 79*).

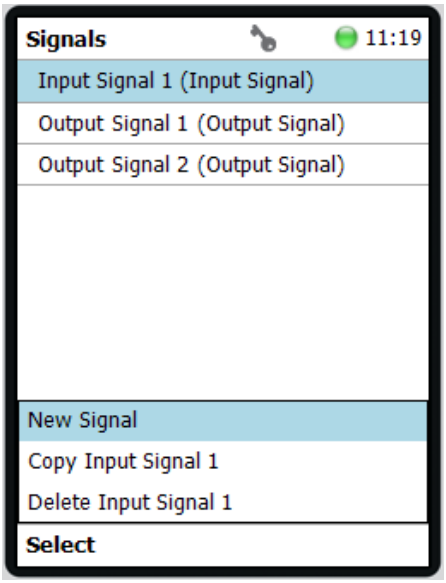


Figure 78 Signals Menu

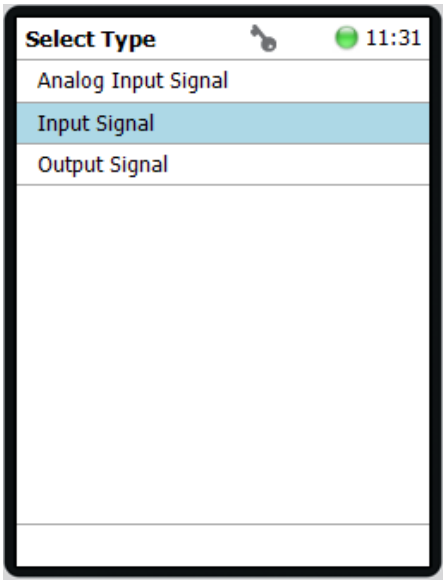


Figure 79 New Signal Menu

When prompted, enter the name “SoftIn”, and press “B” (New) as shown in *Figure 80*.

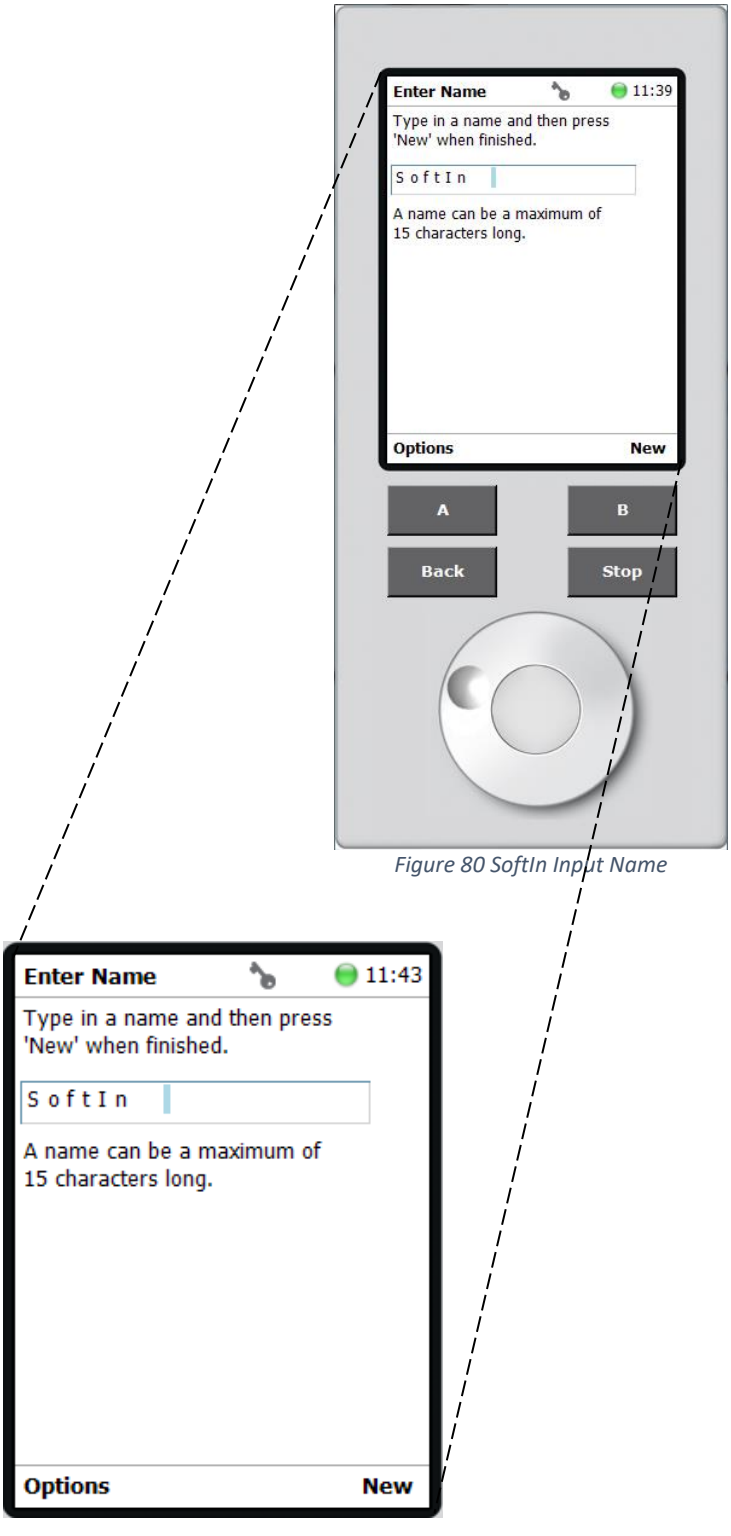


Figure 80 SoftIn Input Name

After creating the new Input Signal “SoftIn”, it is added to the Signals list (*Figure 81)*.

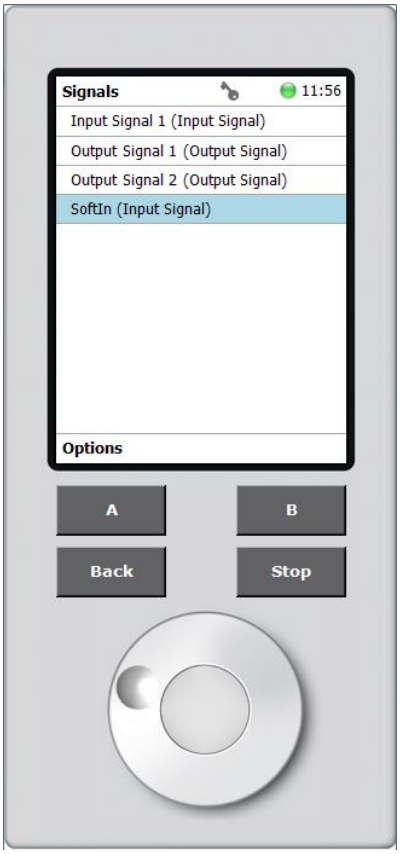


Figure 81 Signal List with SoftIn

Scroll down and select the signal “SoftIn” (Input Signal) to bring up the SoftIn settings menu and change the “Source” setting to Software In (*Figure 82*)

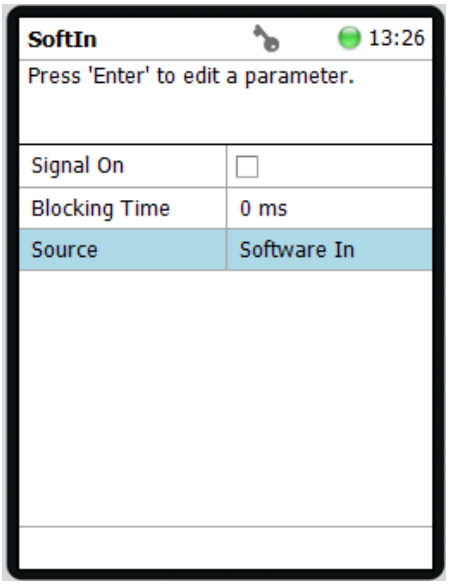


Figure 82 SoftIn Menu

Section 6.6.4.2 – SoftIn Setup

Once the new signal (SoftIn) is created, it has to be assigned to the appropriate Chromatograph System for the Autosampler to recognize the SoftIn software. On the Home Screen, press "A" (Options) to select "Setup" and "PALmodules". In the "PALmodules" menu, select "Chromatogr. Systems" and "GC1 (GC)" (*Figure 83*).

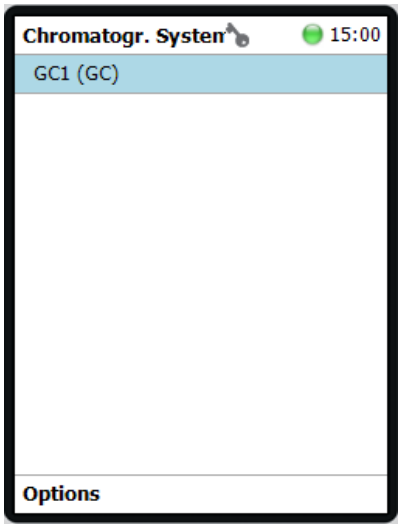


Figure 83 Chromatogr. Systems Menu

In the GC1 menu (Figure 84), modify the "Ready" setting to "SoftIn" using the drop-down list select. Pressing "Back" to exit out to the "PALmodules" menu.

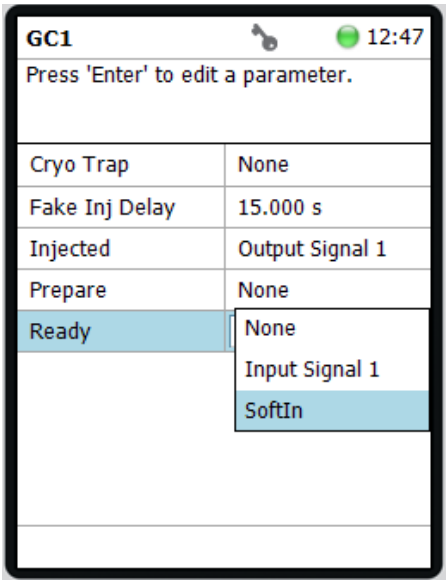


Figure 84 GC1 Settings

Section 6.6.5 – Tray Holder Setup

Tray Holders are used to place sample vials used for calibration and sample analysis. The ATOM Tray Holders contain 3 separate Tray Racks each containing 54 vials (*Figure 85*).

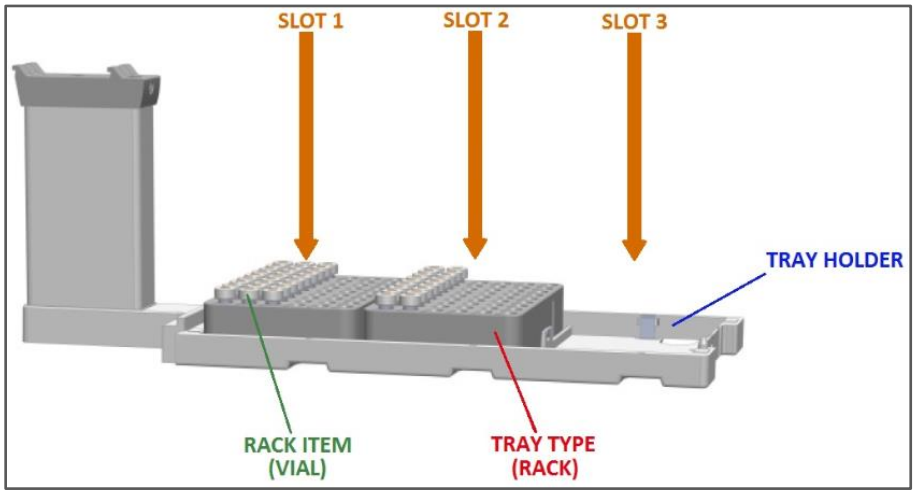


Figure 85 Tray Holder Drawing

Section 6.6.5.1 – Tray Holder Creation

From the Home Screen, press "A" (Options), select "Setup" and "PALmodules". In the PALmodules list (*Figure 86)* select "Tray Holders" and press "A" (Options), to add a "New Tray Holder" (*Figure 87*).

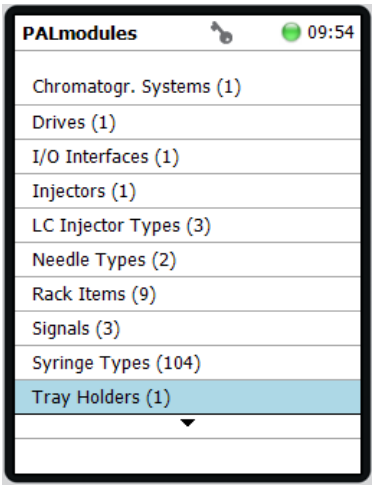


Figure 86 Pal Modules List

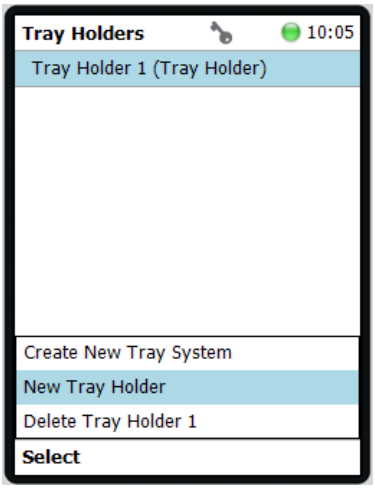


Figure 87 New Tray Holder

Under "Select Type" select "Tray Holder" (*Figure 88*), and when prompted, enter the desired name (*Figure 89*). Press "B" (New) and "Tray Holder 1" will be added to the PALmodules. The ATOM Tray Holder has 3 slots for 3 vial racks which will be defined in the following section.

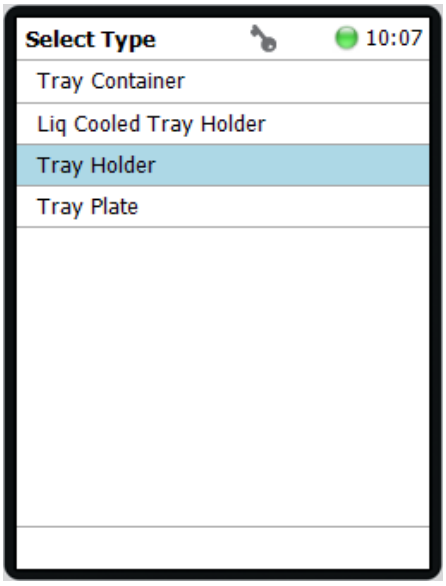


Figure 88 Tray Holder Type Selection

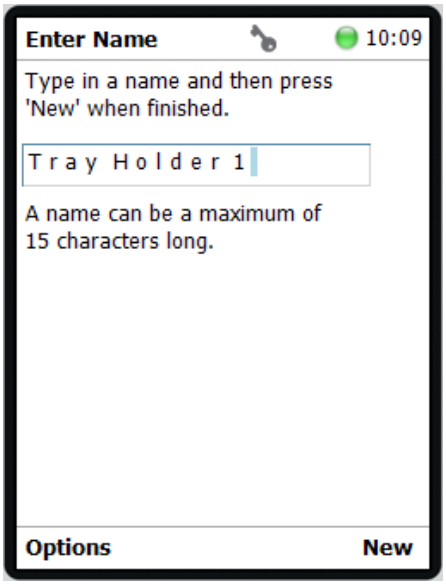


Figure 89 Tray Holder Name Input

Section 6.6.5.2 – Tray Rack Creation

Once the Tray Holder has been created, each individual Tray Rack must be defined. In the Tray Holder section of the PALmodules, open the newly created “Tray Holder 1”. In the Tray Holder 1 menu (*Figure 90*), select “Slot1” and press “A” (Options), to add a “New rack” (*Figure 91*).

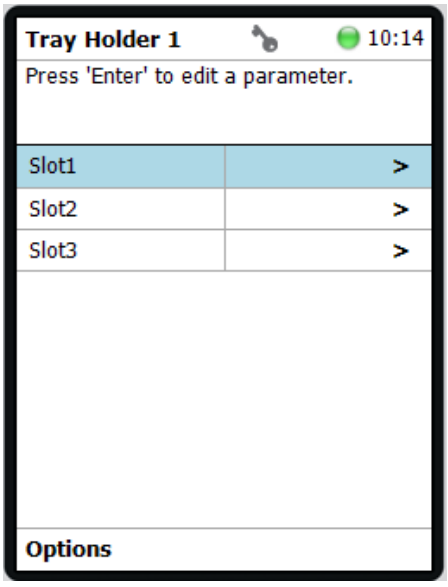


Figure 90 Tray Holder 1 Menu

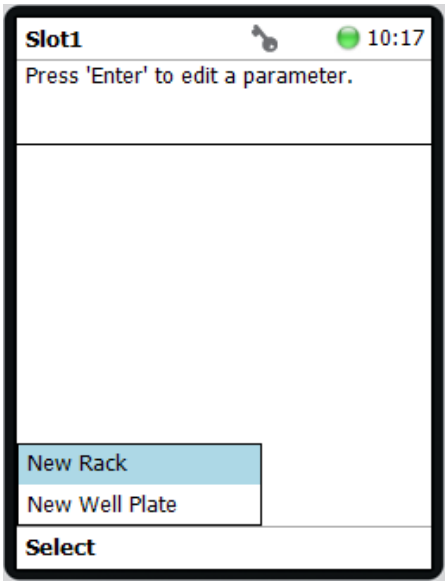


Figure 91 Slot 1 Menu

When prompted, enter the desired rack name (*Figure 92*). Once completed, press “B” (New) and the new rack will be added to “Tray Holder 1”.

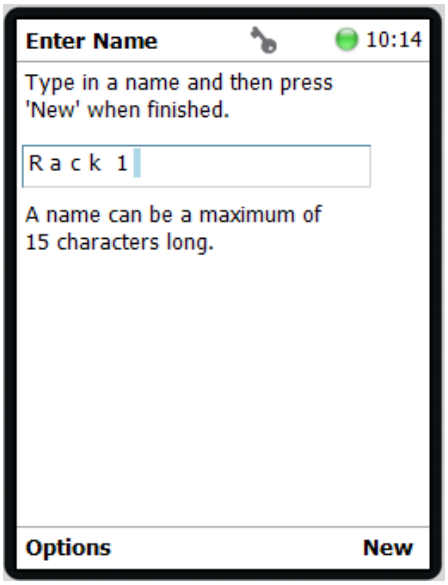


Figure 92 New Rack Name

Once created, select the new rack to bring up the rack menu to adjust the rack parameters. First , modify the “Rack Type” to “VT54” to indicate a 54-vial rack (*Figure 93*), then modify the “Rack Item” to “2-CV NonMagnetic” (*Figure 94*). The “CapType” will automatically change to “NonMagneticCap”.To exit, press “Back” until exiting to the tray holder menu.

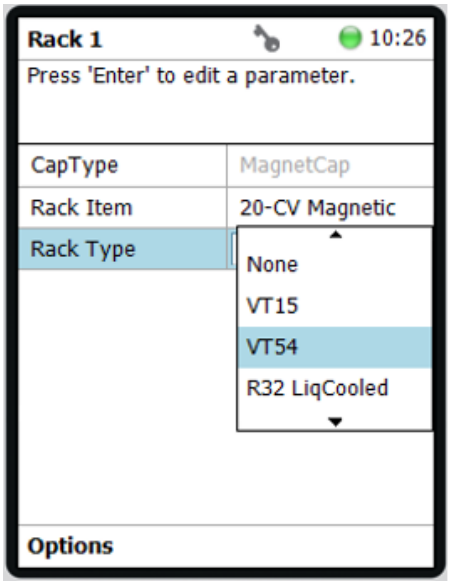


Figure 93 Rack Type Selection

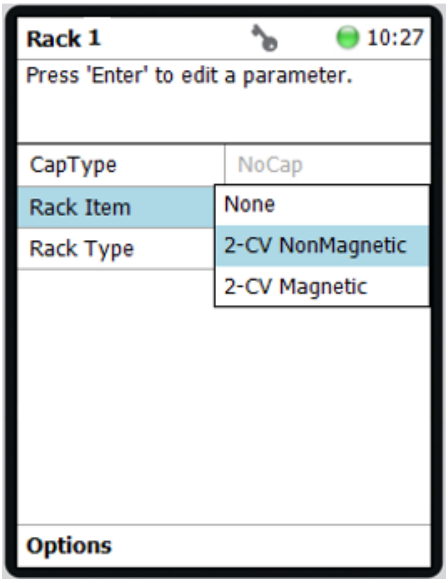


Figure 94 Rack Item Selection

Please note that the procedure must be followed in the order described in this manual. If the recommended order is not followed, some of the default parameters will not load, leading to incorrect configuration.

Repeat the procedure to program the other Tray Holder slots: “Slot2 -> Rack2” and “Slot3 -> Rack3” (*Figure 95*).

Figure 95 Tray Holder Slot Definition

This completes the Tray holder setup. To exit, press the “Back” button until returning to the Home Screen.

Section 6.6.6 – Wash Module Setup

Wash Modules (*Figure 96*) are used to wash the autosampler syringe between the various operations of the autosampler. Wash Modules also contains a waste port used to dispose of the various liquids discarded during the analysis cycle. The ATOM Wash Module consists of 3 elements, two wash vials and a waste port. Wash vials can be used to store solvent (ATOM Instrument recommends using HPLC grade Iso-Octane) or as waste for users wishing to preserve product sent to waste. The waste port is used to discard into a separate container (not provided by ATOM Instrument) the liquids sent to waste.

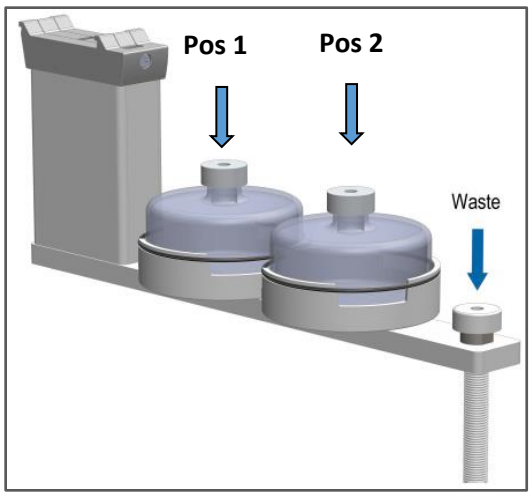


Figure 96 Wash Module Drawing

To setup a Wash Module, press "A" (Options) on the Home Screen and "Setup", to access the "PALmodules" menu (*Figure 97*).

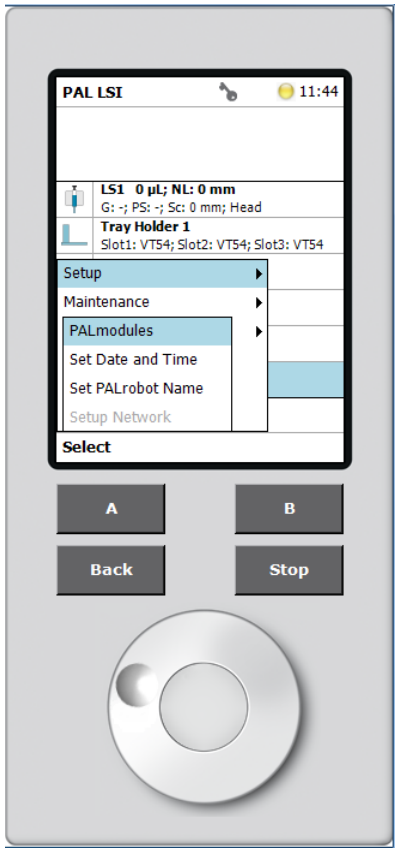


Figure 97 PALmodules Menu

In the PALmodules menu, scroll down to select "Wash Modules" (*Figure 98*) and press "A" (Options) to add a "New Wash Module" (*Figure 99*).

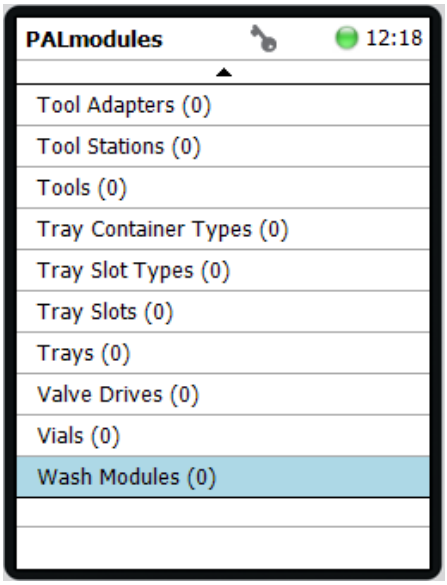


Figure 98 PALmodules Menu

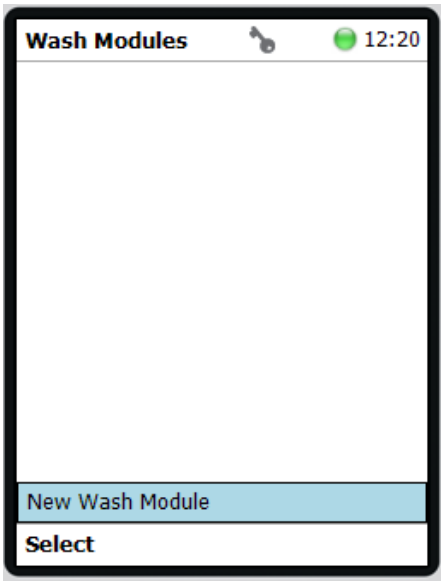


Figure 99 Wash Modules Menu

In the wash modules types list (*Figure 100*), select “Large Wash Module” and when prompted, enter the desired name (*Figure 101*). Press “B” (New) to create the new wash module.

Figure 100 Wash Modules Types

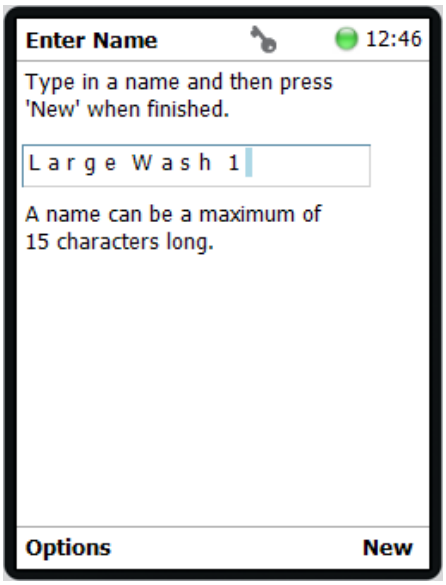


Figure 101 Wash Module Name

Once created, a new Wash Module, will be added to the Wash Modules list (*Figure 102*).

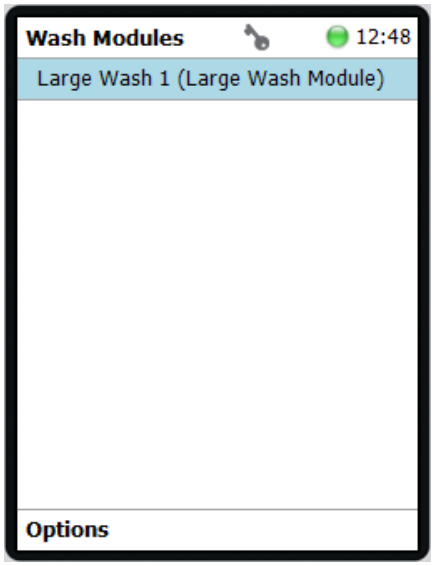


Figure 102 Newly Added Wash Module

Leave all Large Wash module parameter settings to factory defaults (*Figure 103*). Press the “Back” button to return to the Home Screen.

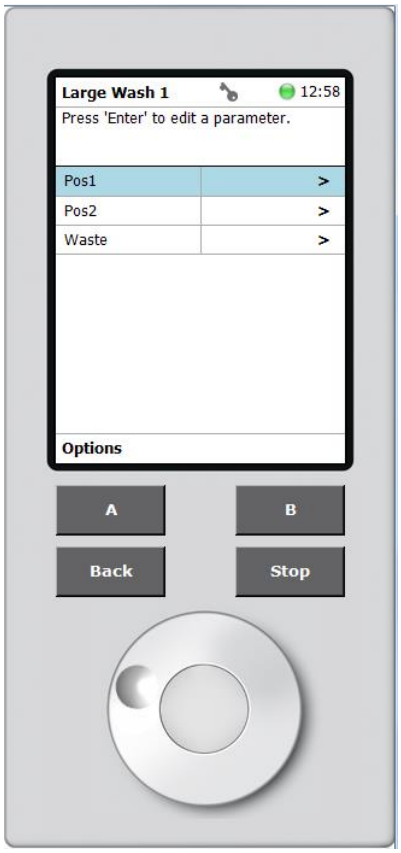


Figure 103 Large Wash Menu

Section 6.6.7 – Injector Setup

The injector represents the location where the autosampler will release the sample in the syringe for analysis.

From the Home Screen, press “A” (Options), select “Setup” and “PALmodules”. In the PALmodules list (*Figure 104)* select “Injectors” and press “A” (Options), to add a “New Injector” (*Figure 105*).

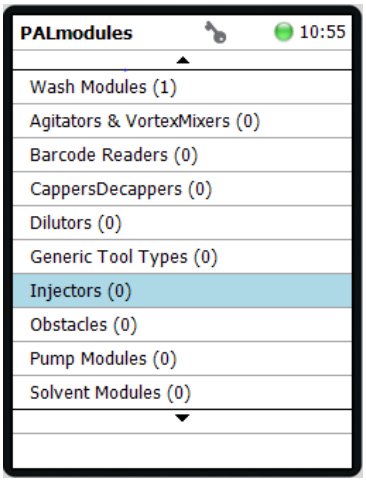


Figure 104 Pal Modules List

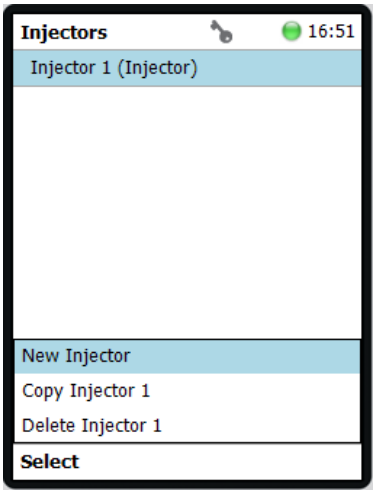


Figure 105 New Injector

Under “Select Type” select “Injector” (*Figure 106*), and when prompted, enter the desired name (*Figure 107*). Press “B” (New) and “Injector 1” will be added to the PALmodules. Once created, leave the default injector settings. To exit, press Back to return to the Home screen.

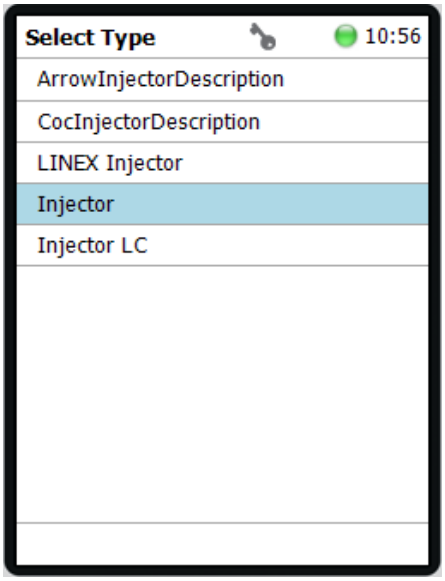


Figure 106 Injector Type Selection

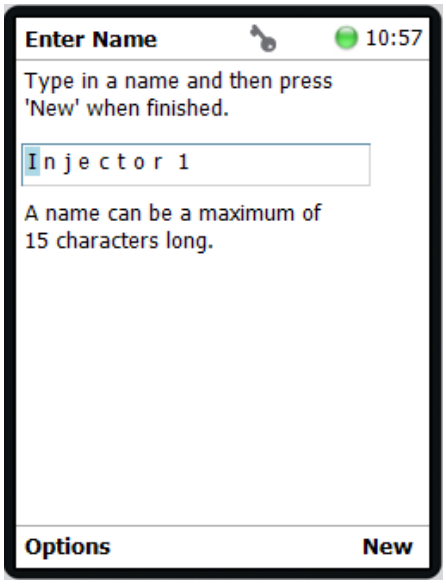


Figure 107 Injector Name Input

Section 6.7 – Modules Teaching

Once the Autosampler assembled and the PALmodules set up, the Autosampler has to be programmed with the physical positions of the PALmodules. This process is referred to as the "Teaching" of PALmodules. This section of the manual covers teaching of the PALmodules defined in the previous section.

Section 6.7.1 – Tray Holder

Tray holders are taught in two steps. The Tray Holder module itself is taught first and then each individual Tray Rack.

Section 6.7.1.1 – Tray Holder Module Teaching

On the "Start Screen", scroll down and select "Tray Holder 1" (*Figure 108*).

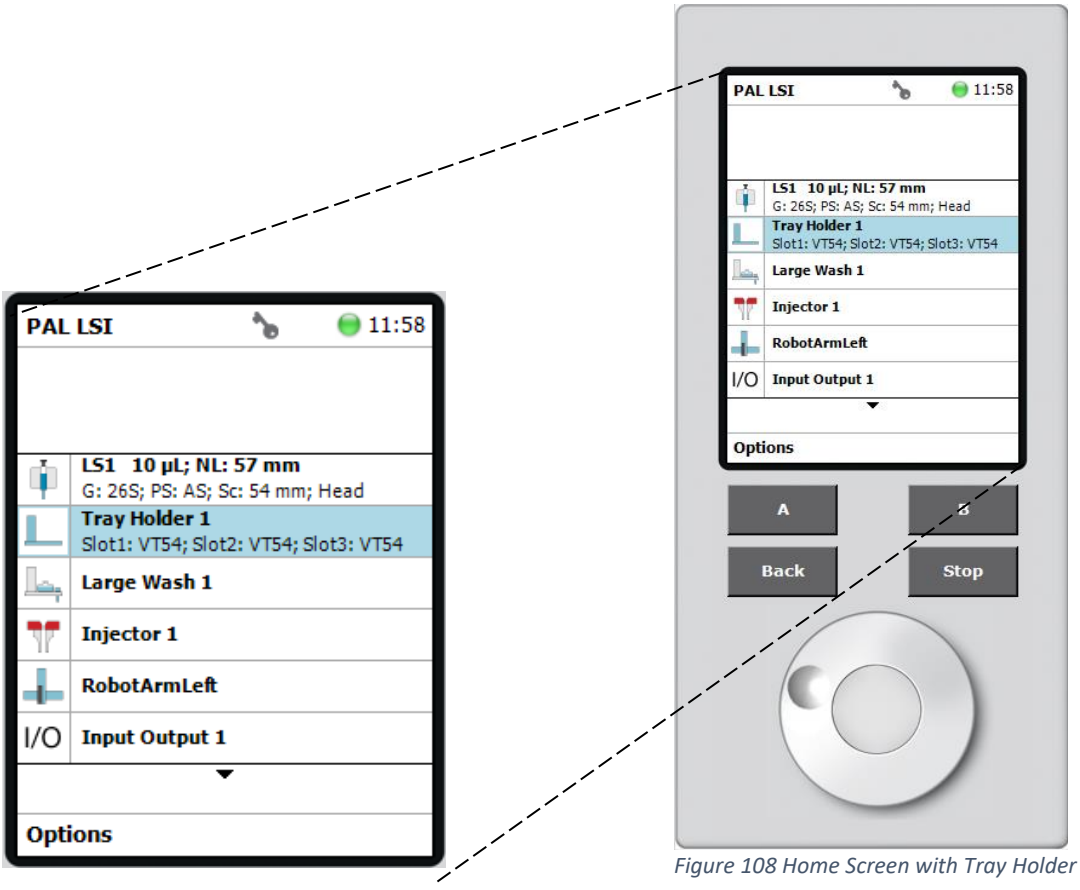


Figure 108 Home Screen with Tray Holder

In the Tray Holder menu, press “A” (Options) and select, in the subsequent menu, “Teach PALmodule” (*Figure 109*) to teach the position of the Tray Holder.

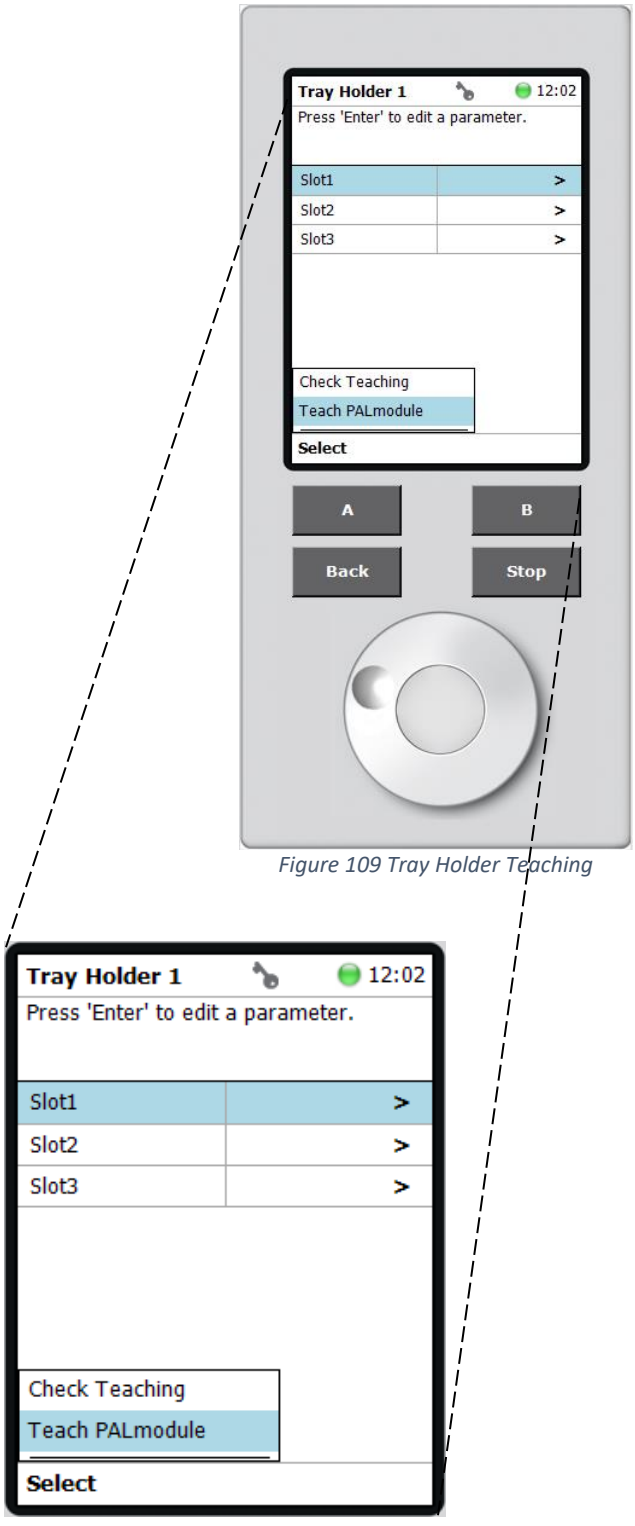


Figure 109 Tray Holder Teaching

Upon selecting Teach PALmodule, the LED light indicator on the autosampler will turn blue to indicate that it is safe to move the PALhead to the position shown on the PAL Terminal (*Figure 110*).

Figure 110 Tray Holder Teaching

Once positioned, the Autosampler will update the X, Y and Z position settings as shown in *Figure 111*. To continue, Press “B” (Next) to enable the fine tuning menu. In the fine tuning menu, select the desired axis to move the PALhead in 0.1 mm increments by scrolling up/down.

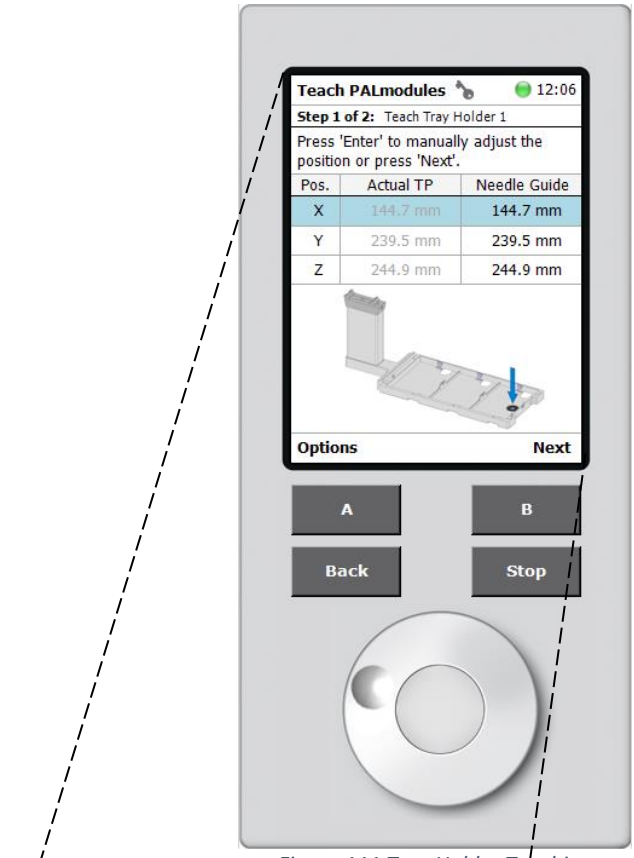


Figure 111 Tray Holder Teaching

Once fine-tuned, press “B” (OK) to move the PALhead to the Home position (*Figure 112*).

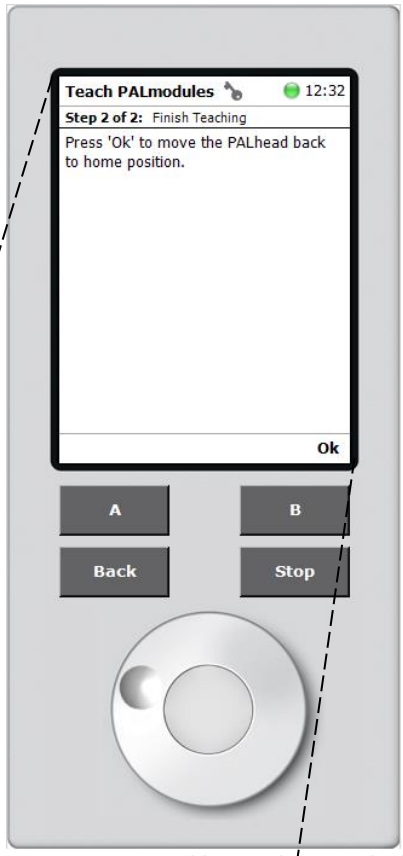
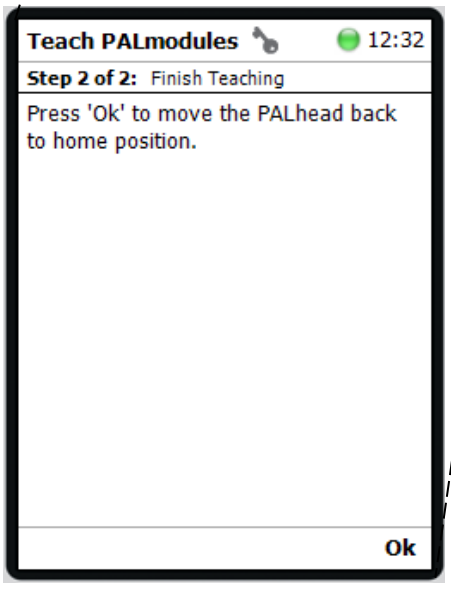


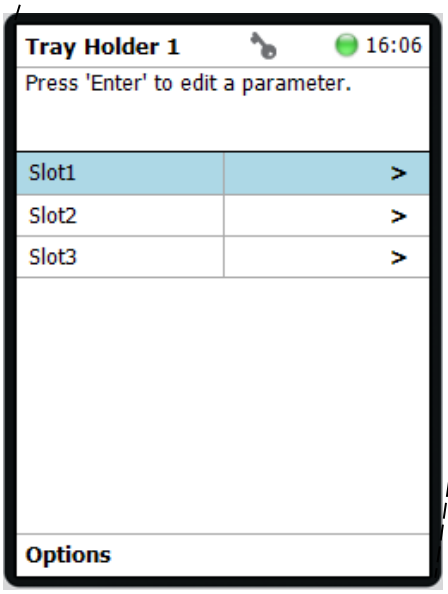
Figure 112 Tray Holder Teaching Finished



Section 6.7.1.2 – Tray Rack Teaching

Once the Tray Holder module taught, each individual Tray Rack must be taught. On the Tray Holder menu select “Slot1” as shown below in *Figure 113*.

Figure 113 Tray Holder Menu



In the Slot 1 menu, select “Rack 1” (*Figure 114*) to open the Rack 1 settings.

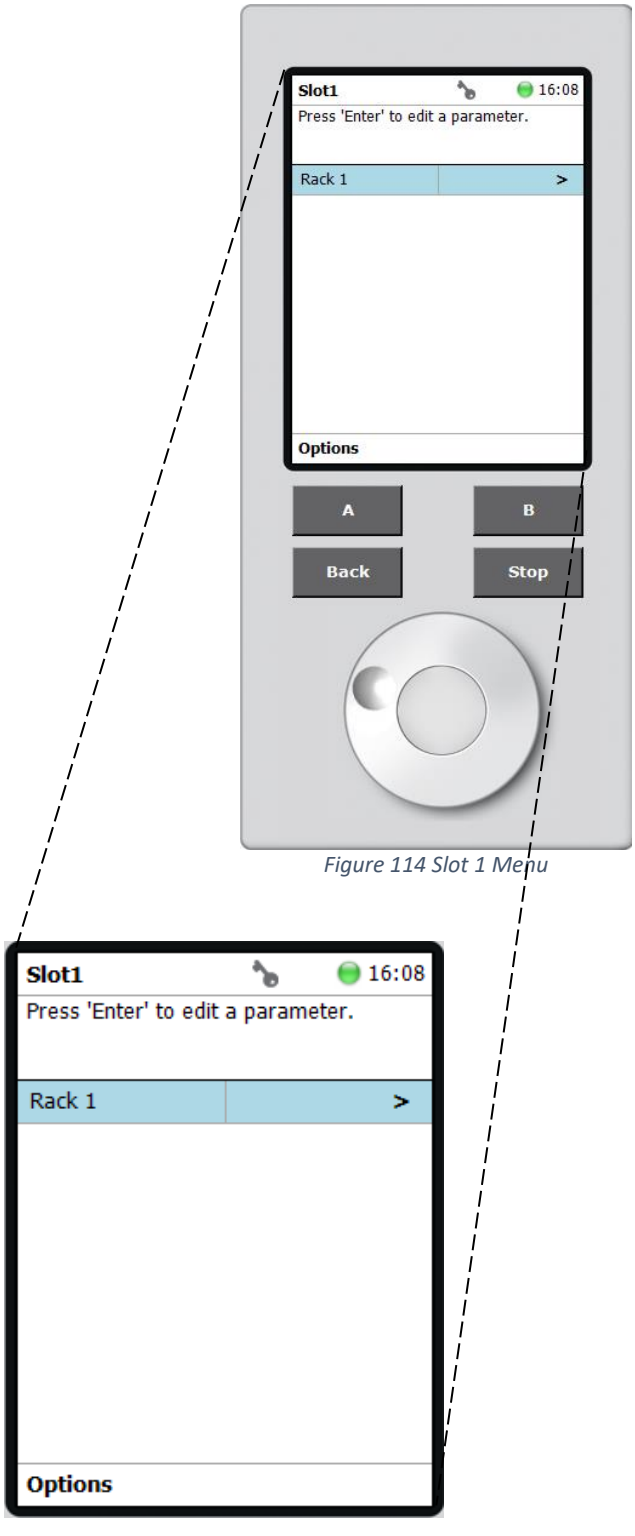


Figure 114 Slot 1 Menu

In the Rack 1 menu, select “A” (Options) and “Teach PALmodule” (*Figure 115)*.

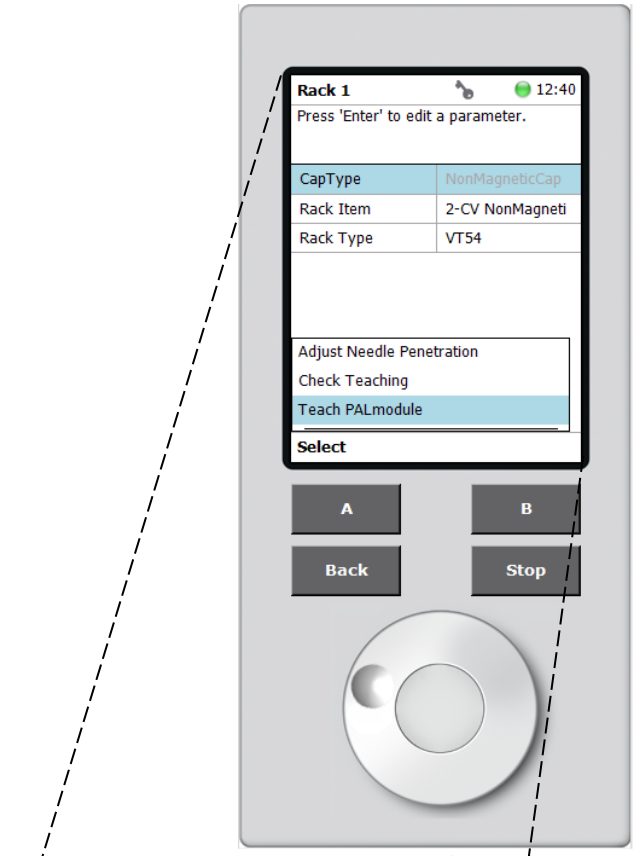


Figure 115 Rack 1 Teaching

To start, place a vial in the rack position 1 shown below (*Figure 116*). When the LED indicator on the autosampler indicates blue, physically move the PALhead over the vial cap (XY axes adjustment), vertically position it slightly above the vial cap and press “B” (Next). In the fine tuning menu, select the desired axis to move the PALhead in 0.1 mm increments by scrolling up/down. Once finished, press “B” (Save) and “B” (Next).

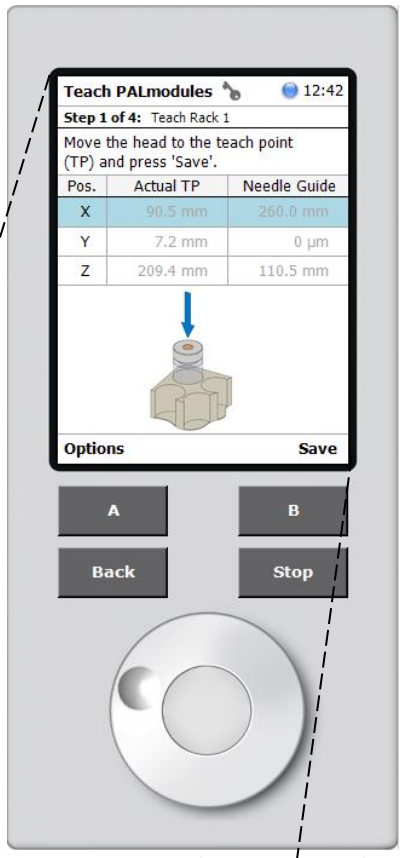
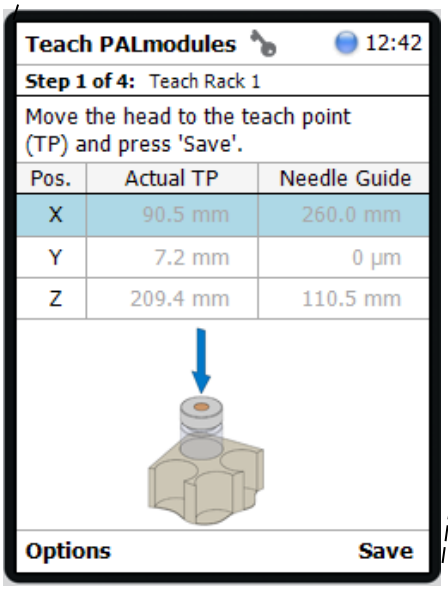
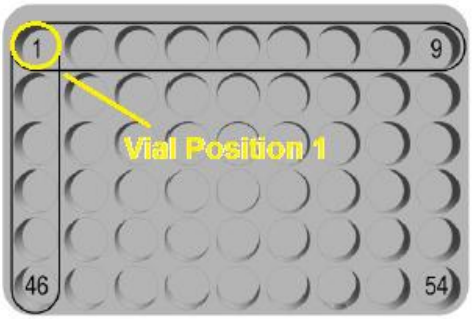


Figure 116 Tray Rack Position 1 Teaching





Tray Type VT54

Place a vial in the rack position 46 shown below (*Figure 117*). When the LED indicator on the autosampler indicates blue, physically move the PALhead over the vial cap (XY axes adjustment), vertically position it slightly above the vial cap and press “B” (Next). In the fine tuning menu, select the desired axis to move the PALhead in 0.1 mm increments by scrolling up/down. Once finished, press “B” (Save) and “B” (Next).

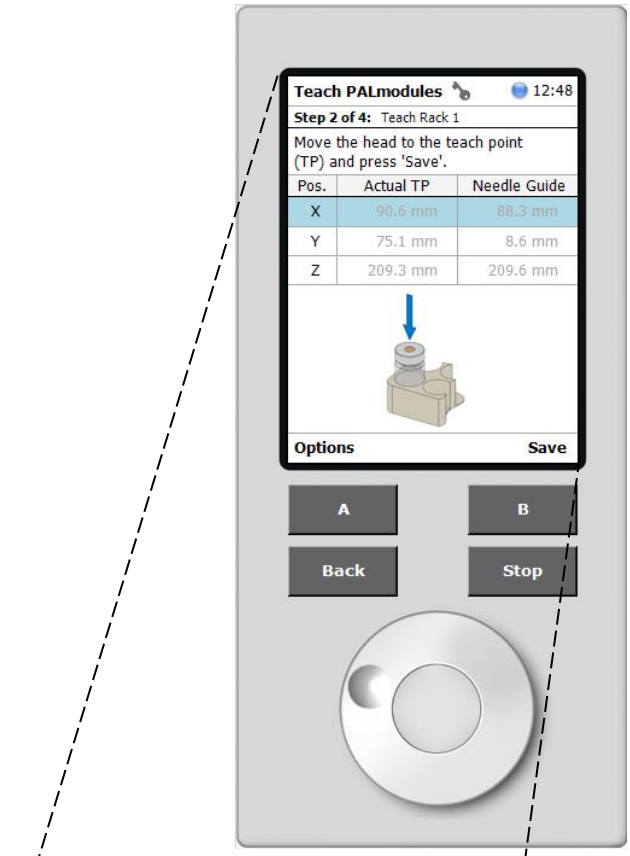
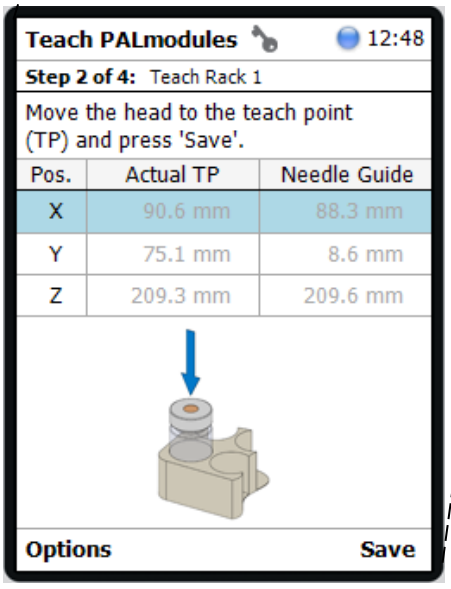
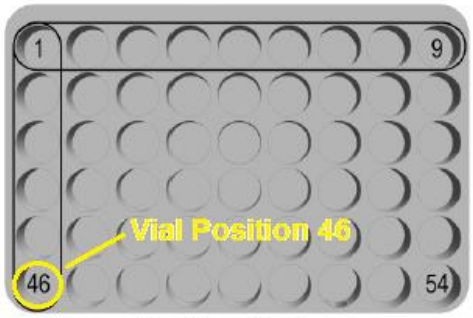


Figure 117 Tray Rack Position 2 Teaching





Tray Type VT54

Place a vial in the rack position 54 shown below (*Figure 118*). When the LED indicator on the autosampler indicates blue, physically move the PALhead over the vial cap (XY axes adjustment), vertically position it slightly above the vial cap and press “B” (Next). In the fine tuning menu, select the desired axis to move the PALhead in 0.1 mm increments by scrolling up/down by scrolling up/down. Once finished, press “B” (Save) and “B” (Next).

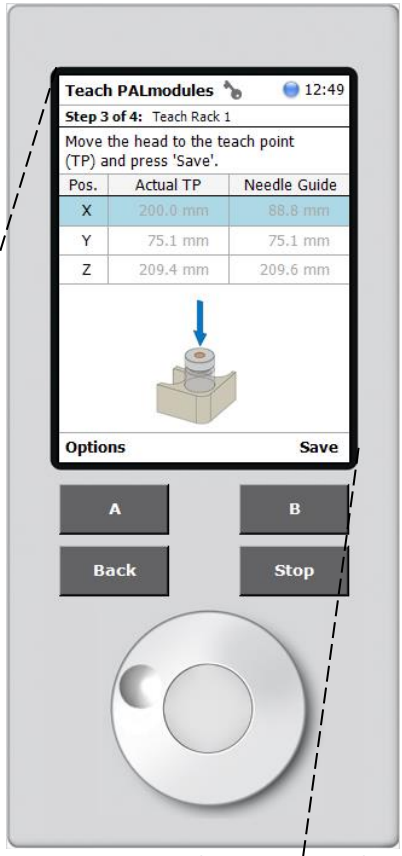
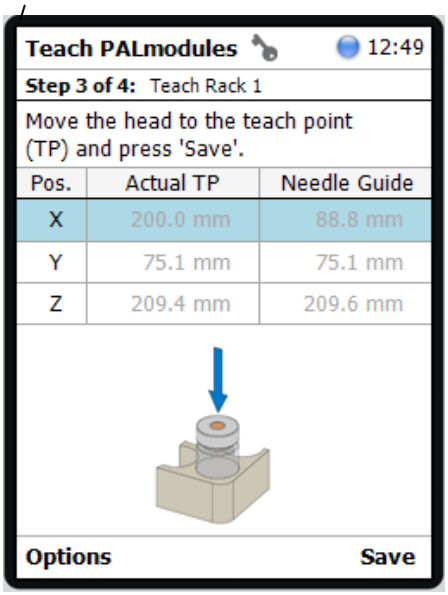
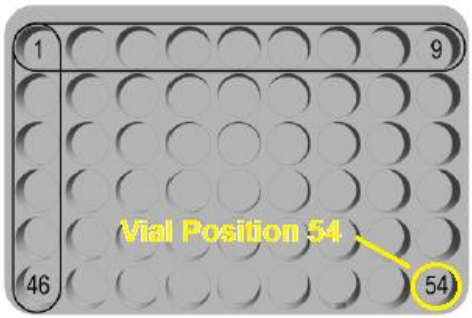


Figure 118 Tray Rack Position 3 Teaching





Tray Type VT54

Once the teaching of all three vial positions for the tray is complete (Step 4 of 4 of *Figure 119*), press “B” (OK) to bring the PALhead back to the “Home” position.

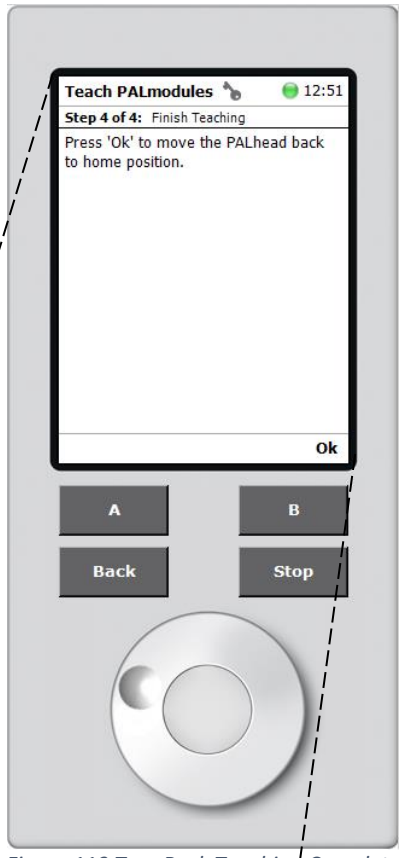
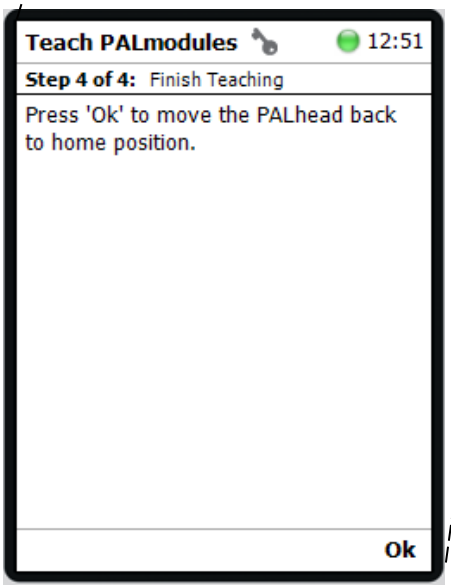


Figure 119 Tray Rack Teaching Complete



Press the “BACK” button until the “Tray Holder 1” menu is reached.

Repeat the above steps to teach Rack 2 and Rack 3 from the respective Slot 2 and Slot 3 (*Figure 120*).

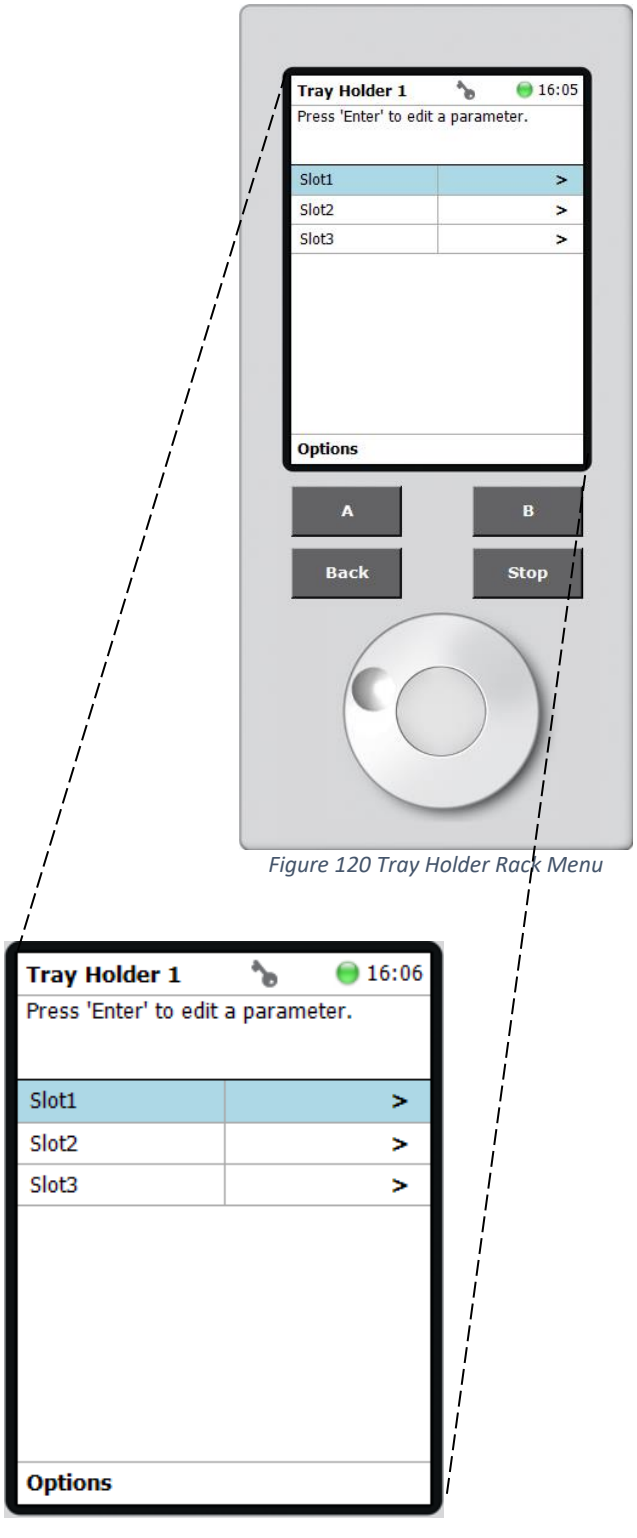


Figure 120 Tray Holder Rack Menu

Once all three Racks are programmed, press the “BACK” button until reaching the Home Screen.

Section 6.7.2 – Large Wash

The Large Wash is taught in two steps. The Large Wash module itself is taught first and then each individual was stations and waste port.

Please note that the "Waste" module position, is used by the Autosampler to record the position of the Wash Station as a whole, and is separate from the individual module positions. Each is covered in the corresponding section.

Section 6.7.2.1 – Large Wash Module Teaching

On the "Start Screen", scroll down and select "Large Wash 1" (*Figure 121*).

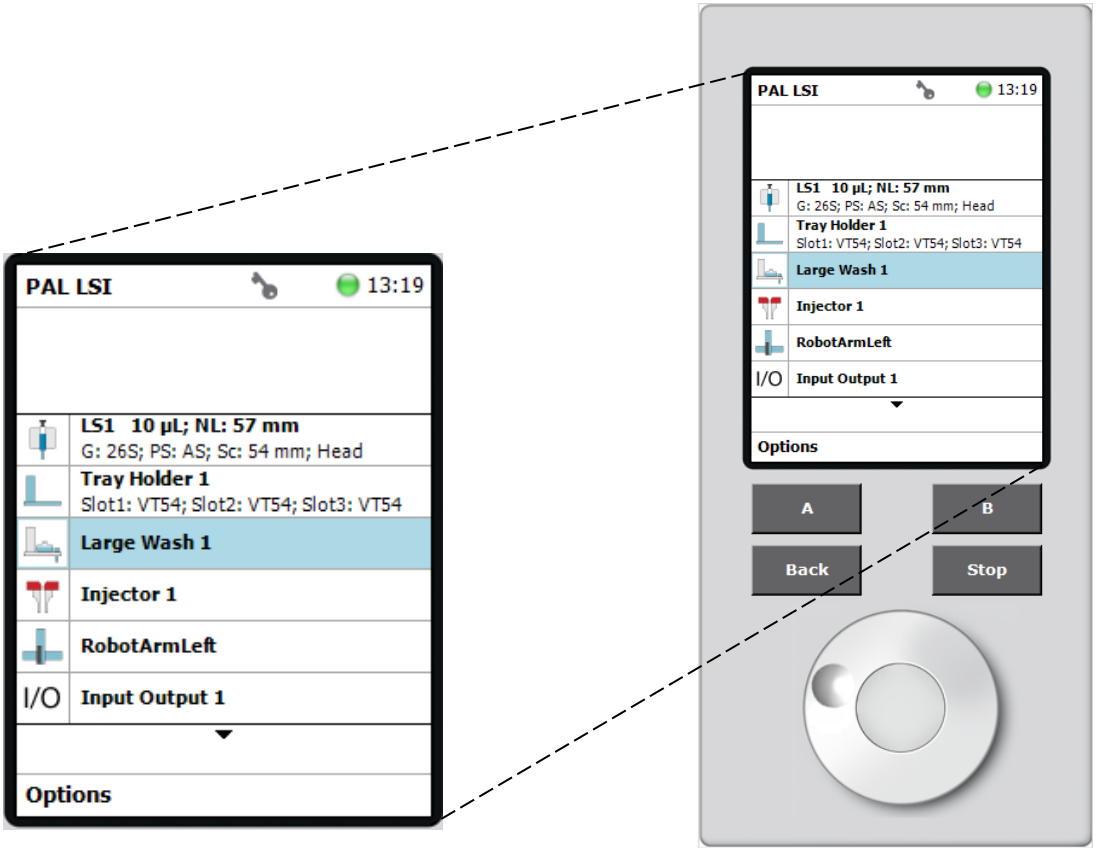


Figure 121 Home Screen Large Wash Selection

Select “A” (Options) and “Teach PALmodule” (*Figure 122*).

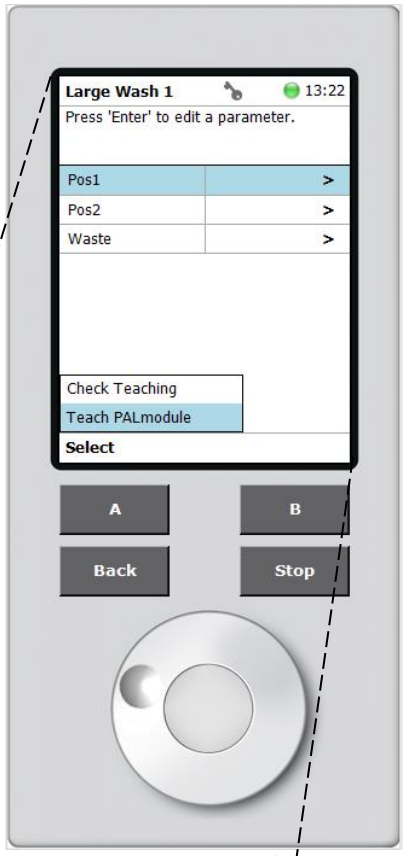
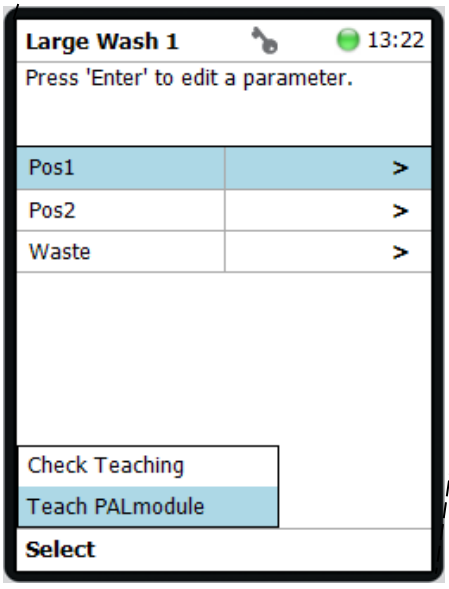


Figure 122 Large Wash Menu



Upon selecting Teach PALmodule, the LED light indicator on the autosampler will turn blue to indicate that it is safe to move the PALhead to the position shown on the PAL Terminal (*Figure 123*). Once positioned, the Autosampler will update the X, Y and Z position settings. To continue, Press “B” (Next) to enable the fine tuning menu. In the fine tuning menu, select the desired axis to move the PALhead in 0.1 mm increments by scrolling up/down. When aligned at the desired position, press “B” (Save).

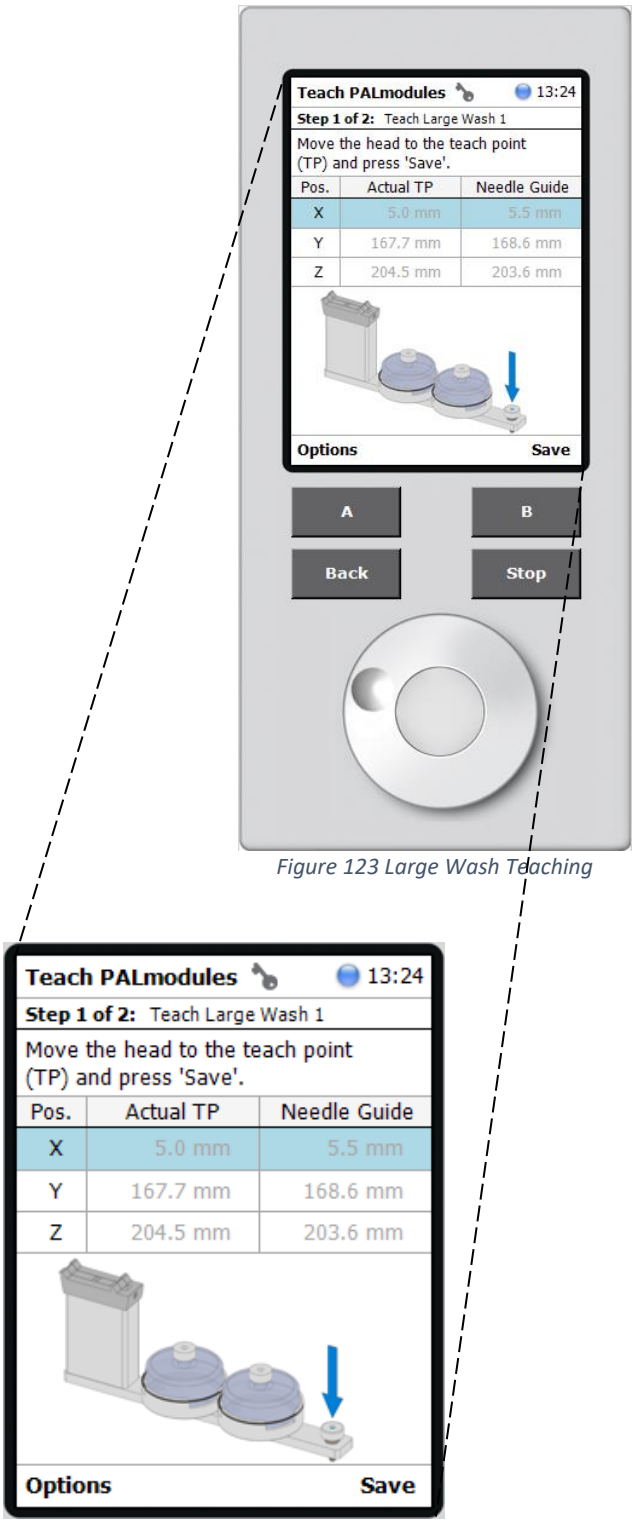


Figure 123 Large Wash Teaching

When prompted press “B” (OK) to return the PALhead to the “Home” position, and exit to the Large Wash menu (*Figure 124*).

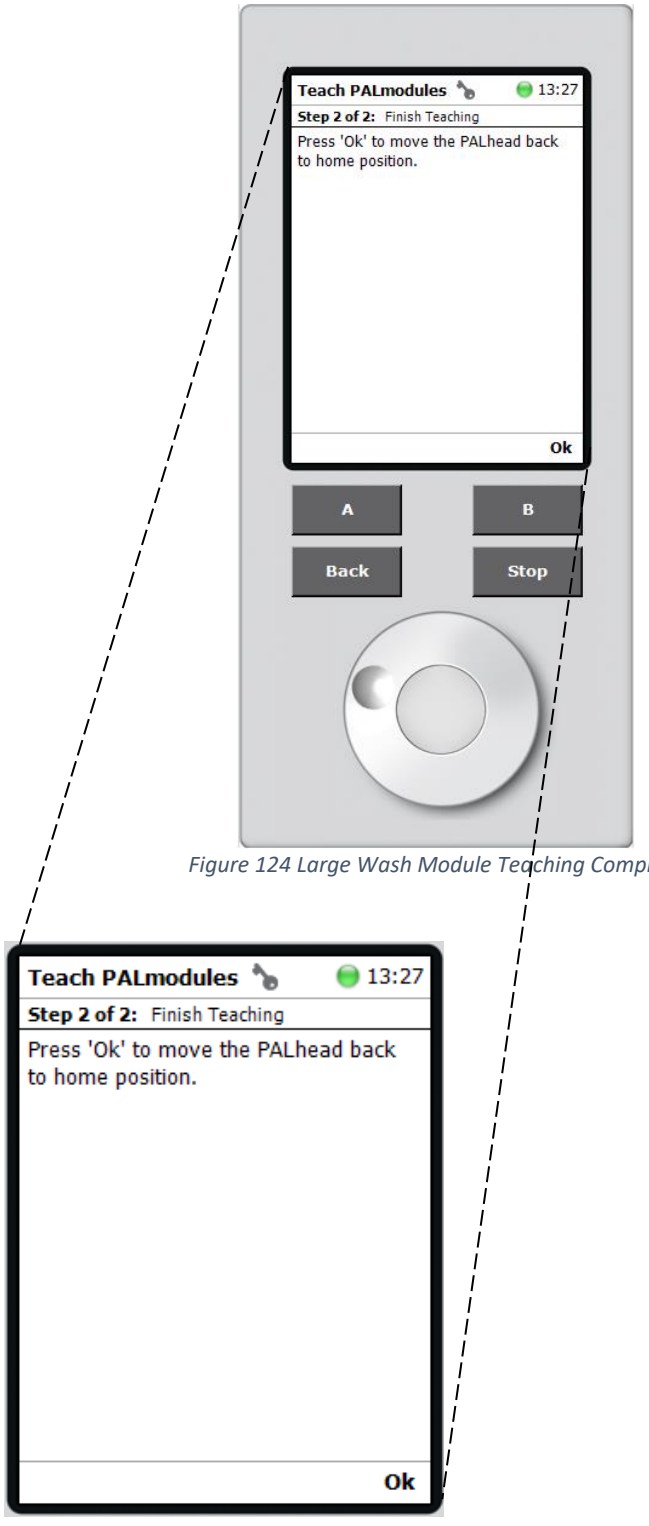
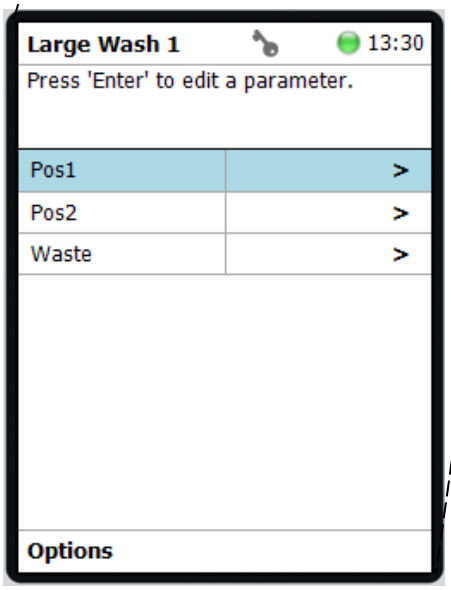


Figure 124 Large Wash Module Teaching Complete

Section 6.7.2.2. – Wash Vials Teaching

Once the Large Wash is taught, the two “Large Wash Vials” at “Pos1” and “Pos2” and the “Waste Port” must be taught. In the Large Wash menu, select “Pos1” (*Figure 125*).

Figure 125 Large Wash Menu



Press “A” (Options), and select “Teach PALmodule” (*Figure 126*).

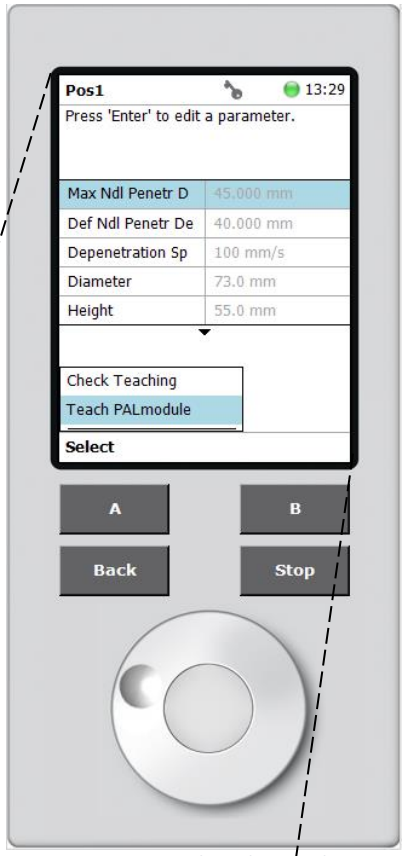
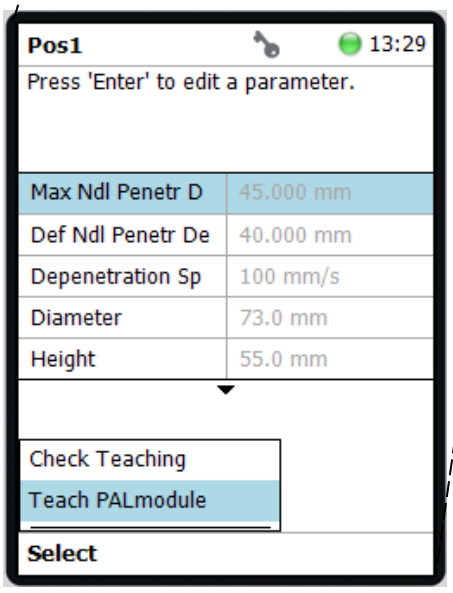


Figure 126 Wash Vial 1 Teaching



When the LED indicator on the autosampler indicates blue, physically move the PALhead over the wash vial port (XY axes adjustment), vertically position it slightly above the wash vial cap and press “B” (Next). In the fine tuning menu, select the desired axis to move the PALhead in 0.1 mm increments by scrolling up/down. When the module is aligned at the desired position, press “B” (Save) (*Figure 127*).

Figure 127 Wash Vial Teaching

When prompted, press “B” (OK) to move the PALhead to back to the “Home” position, and exit to the Large Wash menu (*Figure 128*).

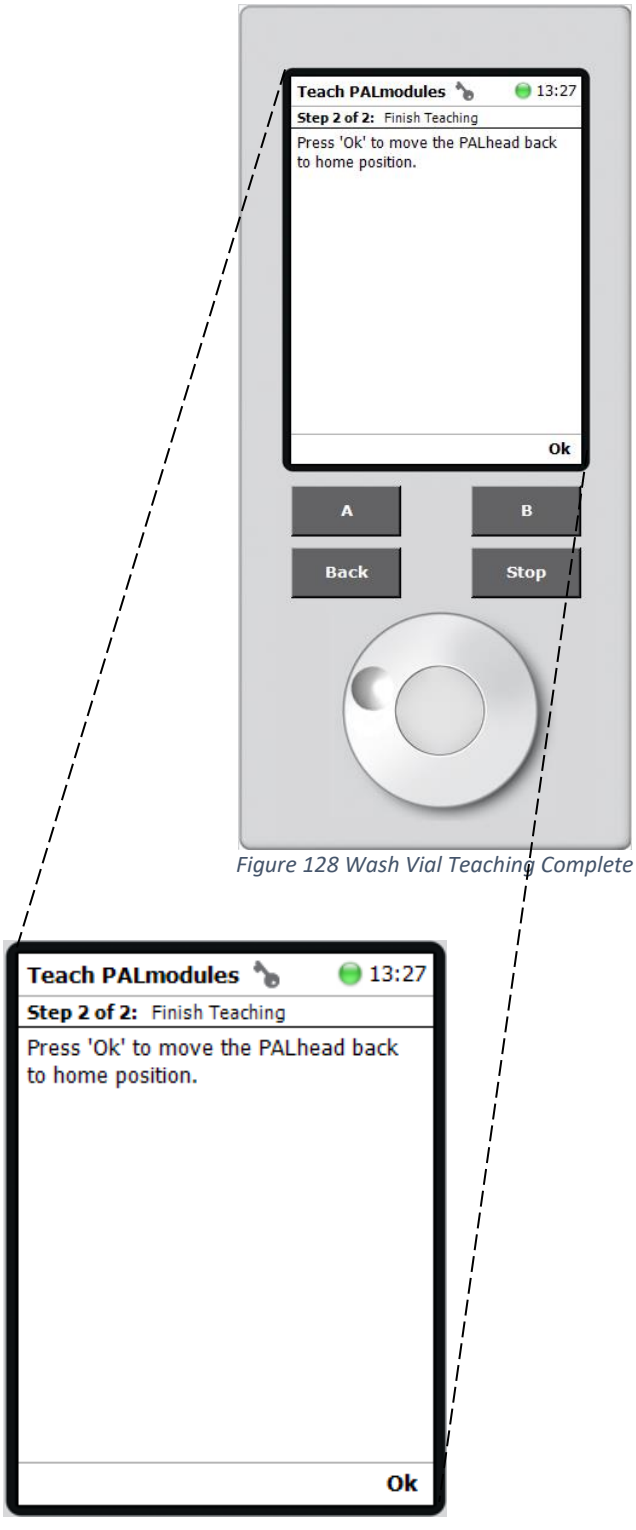


Figure 128 Wash Vial Teaching Complete

Repeat the procedure to teach “Pos2” for the second wash vial.

Section 6.7.2.3 – Waste Port Teaching

Once the Wash Vials are programmed, press the “BACK” button to you exit to the Large Wash menu and select the “Waste” port. In the Waste port menu, press “A” (Options) and select “Teach PALmodule”. When the LED indicator on the autosampler indicates blue, physically move the PALhead over the waste port (XY axes adjustment), vertically position it slightly above the waste port and press “B” (Next). In the fine tuning menu, select the desired axis to move the PALhead in 0.1 mm increments by scrolling up/down. When the module is aligned at the desired position, press “B” (Save) (*Figure 129*).

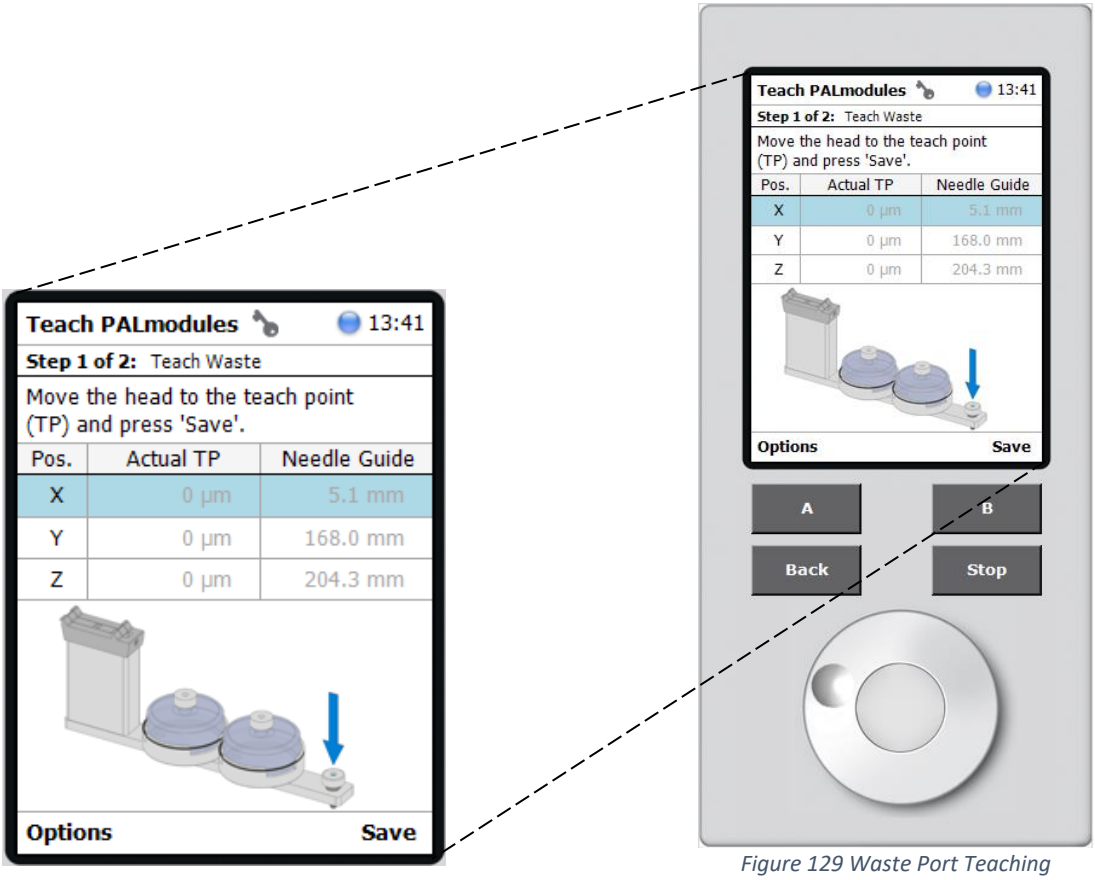


Figure 129 Waste Port Teaching

When prompted press “B” (OK) to move the PALhead back to the “Home” position and exit to the Large Wash menu. Press the “Back” button to exit to the Home Screen (*Figure 130*).

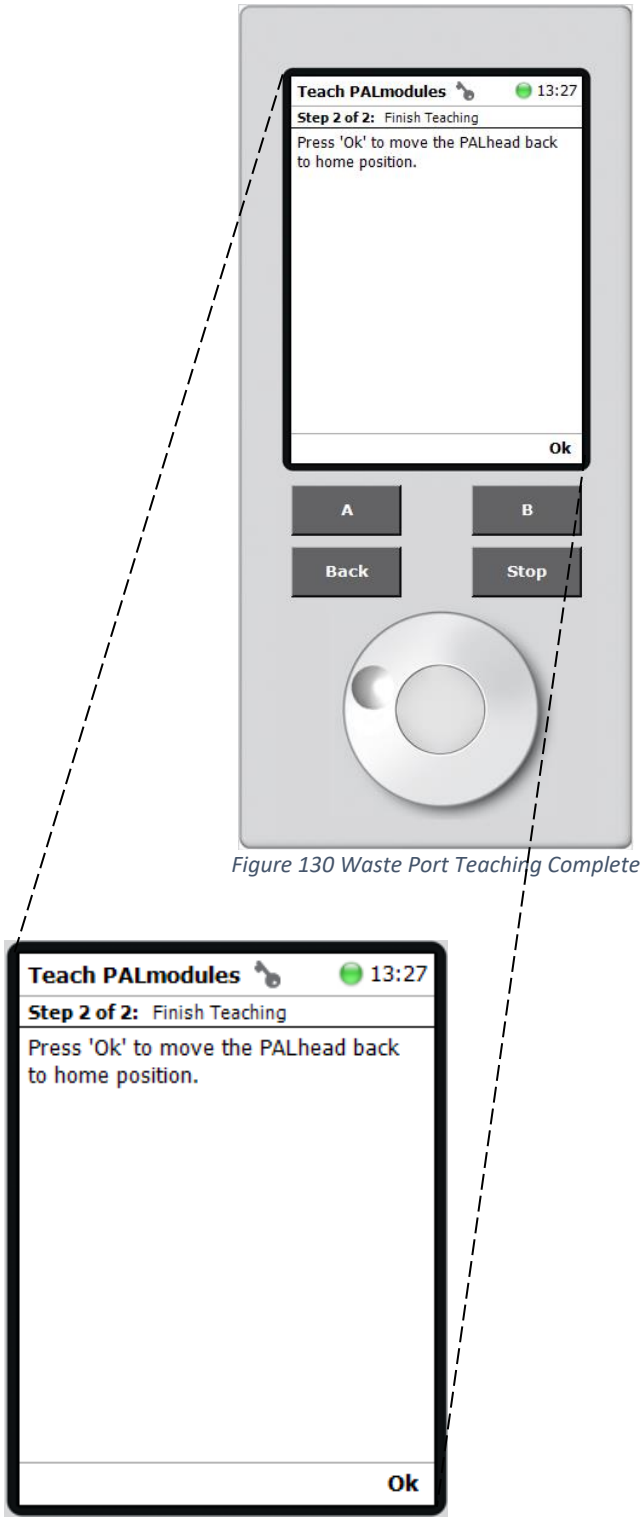


Figure 130 Waste Port Teaching Complete

Section 6.7.3 – Injector Teaching

On the “Start Screen”, scroll down and select “Injector 1” (*Figure 131*).

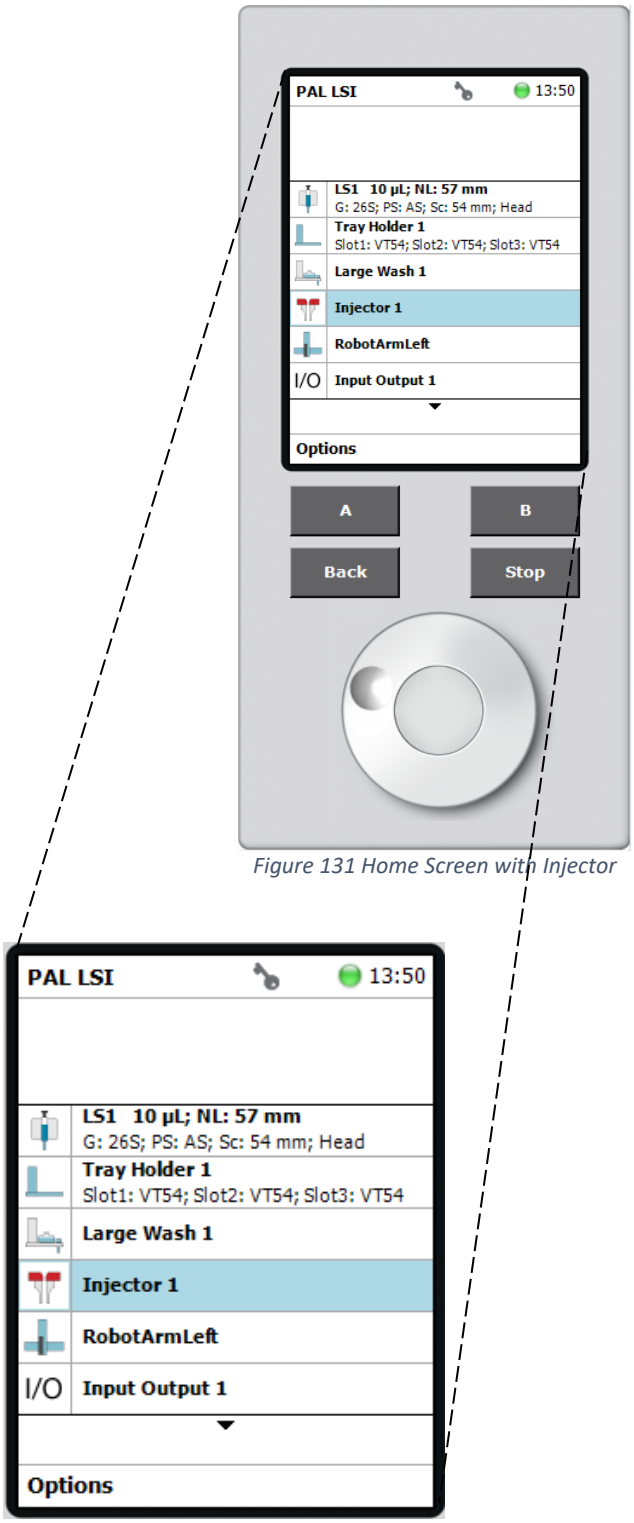


Figure 131 Home Screen with Injector

Press “A” (Options), and select “Teach PALmodule” (*Figure 132*).

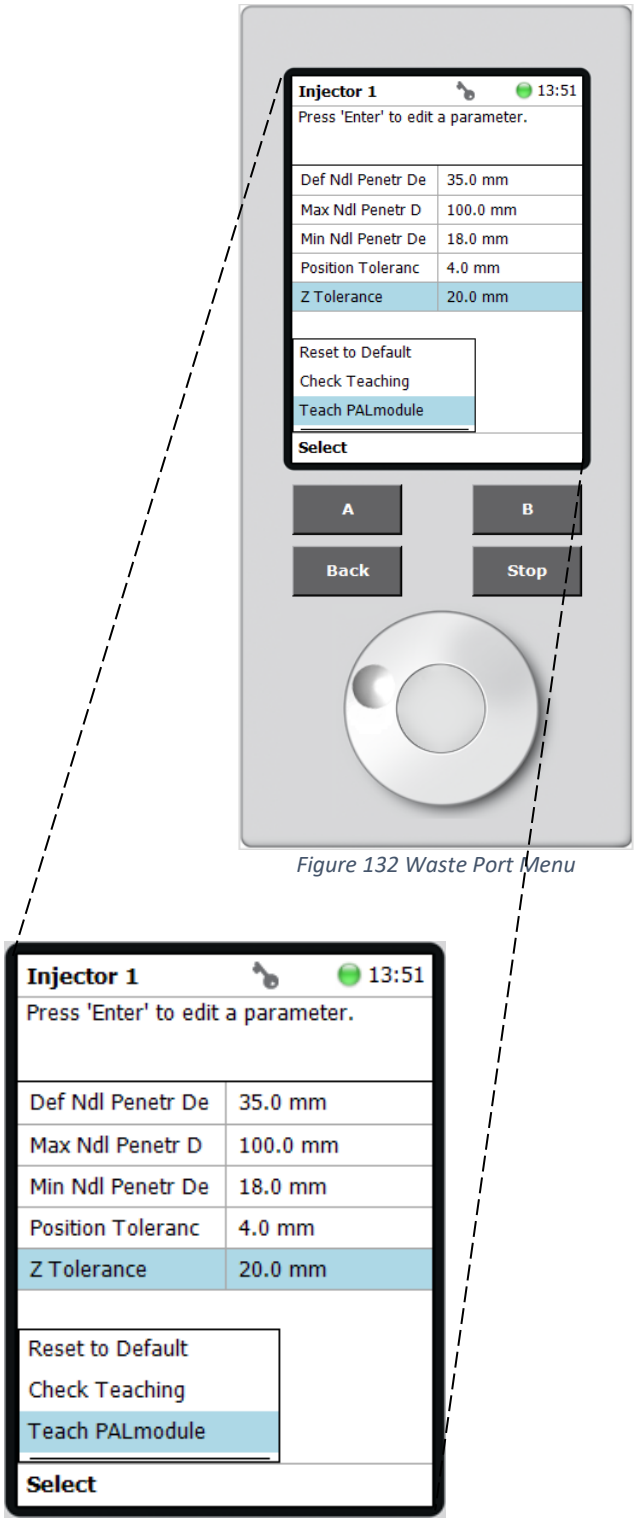


Figure 132 Waste Port Menu

When the LED indicator on the autosampler indicates blue, physically move the PALhead over the injection port (XY axes adjustment), vertically position it slightly above the injection port and press “B” (Next). In the fine tuning menu, select the desired axis to move the PALhead in 0.1 mm increments by scrolling up/down. When the module is aligned at the desired position, press “B” (Save) (*Figure 133*).

Figure 133 Injection Port Teaching

Teach PALmodules 13:53
Step 1 of 2: Teach Injector 1
Move the head to the teach point (TP) and press 'Save'.
Pos. | Actual TP | Needle Guide
X | 349.4 mm | 349.2 mm
Y | 3.4 mm | 3.9 mm
Z | 299.0 mm | 299.6 mm
Options Save

When prompted press “B” (OK) to move the PALhead to the “Home” position and exit back to the Large Wash menu. Pressing the “Back” button to exit to the “Start Screen” (*Figure 134*).

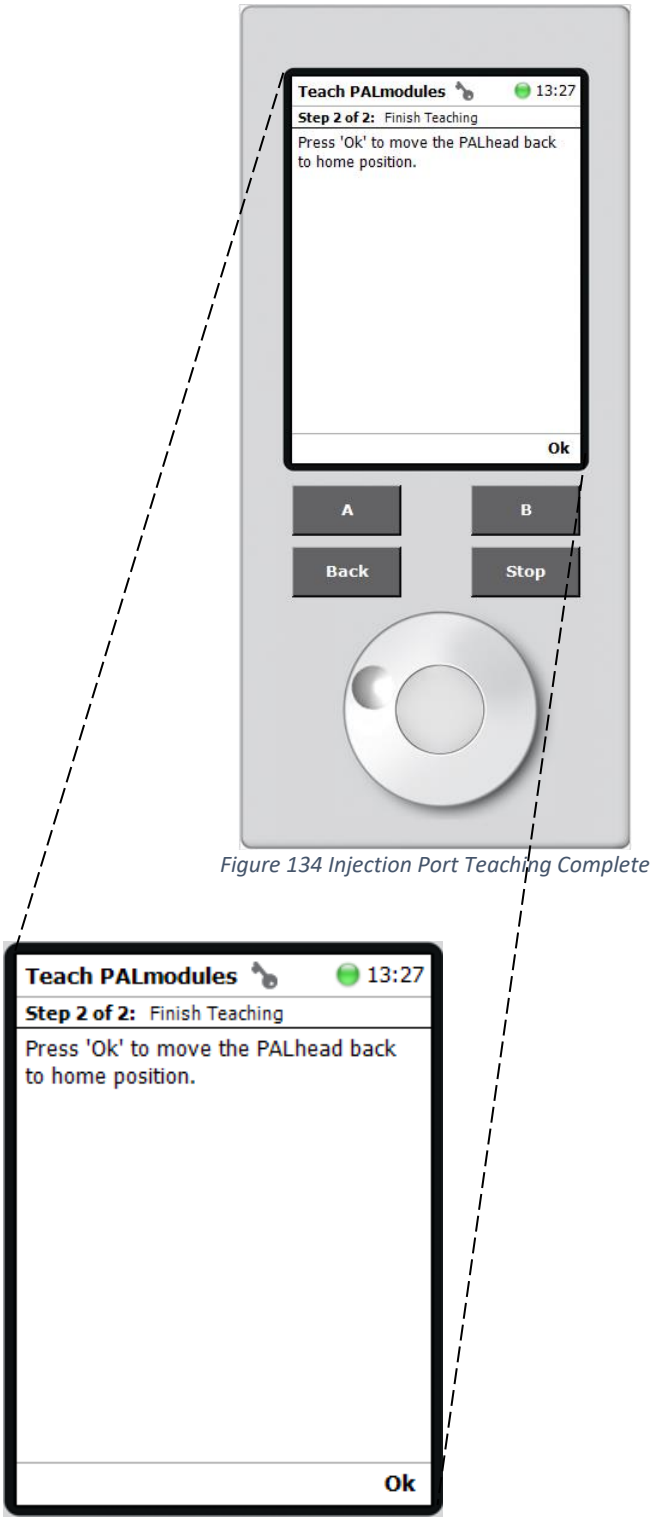


Figure 134 Injection Port Teaching Complete

Section 6.8 – Glossary of Definitions

PALrobot
The term PALrobot is a generic term referring to the PAL System. PALrobot is most often used to refer to the basic unit, meaning the X-Axis, Y-Axis, PALhead and installed PALpower.

PALhead
Refers to the entire injection unit consisting of Z-Axis, the Needle Guide Drive and the Plunger Drive. The cover (PALhead Cover) is also considered as part of the entire unit.

PALmodule
PALmodule is a generic term. It can refer to both “active” and “passive” PALmodules. Syringes, Tray Holders, Wash Stations, are examples of PALmodules.

PALdrive
A “PALdrive” is a generic term for the new generation of “motors” used for the axes. The PALdrive uses the logic of a servo drive with electronic and software control. The various PALdrives are specified using the suffix of where the drive is located, such as PALdrive-X or PALdrive-Z.

PALtool
PALtool is a generic term for the holder of a syringe. Three different PALtools are used: Syringe Tool for liquid sample syringes; Headspace Tool for gaseous sample syringes (Headspace technique) and the SPME Tool for the SPME Fiber technique. A PALtool consists of the lower and upper needle guides, the electronic identification, heating and purge gas connections if required, the coupling pivots for the tool itself and the needle guide. A PALtool is designed for a specific syringe type tailored for the application (liquid, headspace or SPME), with a specific glass barrel outer diameter and needle length.

Tray Holder
A Tray Holder can hold one or more trays. Each Tray Holder has a reference position (X-, Y-, Z-coordinates) that defines its location. A Tray Holder is a passive PALmodule. The type “Tray Holder” can accept a large Rack which spans all three slots, such as the Tray Type “R60”, or three separate Racks in the three slots, such as type “VT54”.

Slot
A “Slot” is defined as a position within a Tray Holder which can be occupied by a Tray. A Tray can be a Rack if vials are used, for example Rack VT54. Tray Holders contain “Slots” for holding Trays. The numbering for Slots is defined from the PALrobot X-Axis to the front. *Figure 118* illustrates the example of a Tray Holder including the Slots with spaces for installing three Racks.

Tray
A tray is generic term. A tray can be a “Rack” for holding vials or a Well Plate for holding Deepwell plates or Microtiter plates. A Tray holds multiple samples. Trays are defined by designating the Tray Type (see below) and the Tray Holder. Tray names are used to identify the sample source within a PAL Job.

Rack

A Tray holding vials is called a “Rack”. A Rack with the same footprint as a Well Plate has the abbreviation “VT” (for example, VT54 as specified earlier on Page 10 of this manual).

VT54	Rack with same footprint as Well Plate; 54 positions (6 x 9); Pattern: Regular for 2 mL vials with OD 12 mm and height 34 mm.

Rack Item

The physical dimensions of Vials that are handled within racks and the parameters required for automation, such as “Needle Penetration Depth” or “Penetration Speed”, are described by the various item parameters of the Rack Item.

Tray Type

A Tray Type is a generic term. A Tray Type can be a “Rack Type” (for vials) or a “Well Plate Type” (for Well plates). The Tray Type defines the pattern and sampling sequence of sample locations within a Tray.

Vial Type

The physical dimensions of Wash Vials and Waste Vials and the parameters required for automation, such as “Needle Penetration Depth” or “Penetration Speed”, are described by the various item parameters of the Vial Type.

Section 7 – External Injection Module

The External Injection Module (EIM) is used to inject Gases and Liquid Hydrocarbons (LPG) into the analyzer. The EIM comes in various configurations depending on the application

This section gives further information about the External Injection module (EIM) and its various components. The diagram below gives an overall idea of the EIM parts

Section 7.1 – Components

There are multiple components in the various models of EIM. All of the components are located inside the EIM enclosure. The components include power supply, valve controllers, valves, mass flow controller and flowmeters. This section will detail some of the major components found in the various EIM models.

Section 7.1.1 – Gas, Liquid/LPG and Sample Shut Off Valves

The EIM contains 2 valve slots, one for the Liquid/LPG valve and one for either the Gas Valve or the Liquid/LPG Sample Shut Off Valve. All 3 valves are identical but programmed differently depending on their use. The valves are 6-port valves actuated electrically and controlled directly by the software. When in use, the Gas valve is built with a 2.5 mL sample loop and the Liquid/LPG valve is built with a 10 uL sample loop.

Section 7.1.2 – Mass Flow Controller

The mass flow controller is used to push the sample from the sample valve to the analyzer. There is one mass flow controller for the entire EIM. When using a Gas and Liquid/LPG EIM, the carrier flow goes through both valves before bringing the sample to the analyzer.

Section 7.1.3 – Sightglass and Flowmeter

Depending on the configuration of the EIM, the liquid/LPG side may have either a Flowmeter (Figure 135) or a Sight Glass (Figure 136). The Sightglass is pressure rated for 1,000 psi (70 bar) whereas the flowmeter is pressure rated at 500 psi (35 bar). An EIM configured for Gas samples will also include a flowmeter on the gas side (Figure 136) pressure rated at 200 psi

Figure 135 EIM with LPG Flowmeter

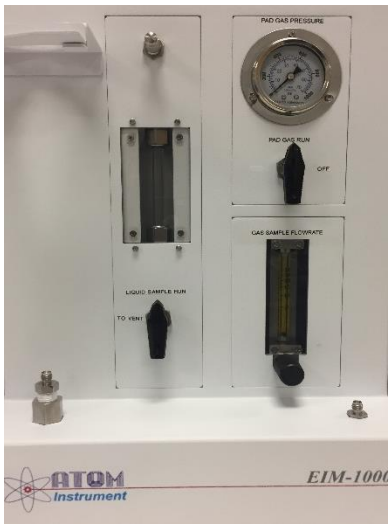


Figure 136 EIM with LPG Sightglass and Gas Capability

Section 7.2 – Models

The External Injection Module (EIM) comes in multiple versions. The table below lists all the available models with their specific configurations.

Model	Liquid Side		Gas Side	
	Sightglass	Flowmeter	Gas Valve	Sample Shut Off
EIM-1000-L	X			
EIM-1000-LF		X		
EIM-1000-LSO	X			X
EIM-1000-LFSO		X		X
EIM-1000-G			X	
EIM-1000-GL	X		X	
EIM-1000-GLF		X	X	

Section 7.3 – Drawings

Section 7.4 – Using the EIM

The EIM is automatically controlled by the LUI software. Sample valves are activated following a sequence predefined depending on the EIM configuration. User intervention is limited to ensure optimal analytical performance. This section will detail how to use an ATOM EIM depending on the intended analysis.

Section 7.4.1 – Gas samples

Section 7.4.1.1 – General Guidelines

When using a Gas EIM without a sample shutoff, the user must first connect the gas sample to the gas inlet of the EIM. The gas flowmeter allows setting the desired flowrate for the analysis. ATOM recommends setting the flow high enough to have sufficient product circulation through the flow path (Total flowpath volume below 5 cc) but not too high to avoid wasting sample. To adjust sample flow, rotate the control valve of the flowmeter counterclockwise to increase flow and clockwise to decrease flow.

Once the flow is properly adjusted, the analysis may be standard and the software will automatically control the EIM and collect data from the detectors to generate a sample peak and compare to stored calibration in the case of a standard or a specific concentration in the case of a standard.

Once all runs within a samples have been analyzed, the software will prompt the user to load the next sample if other samples remain or finish the sample set if the last run has been performed.

Section 7.4.1.2 – Procedure

To run a gas sample on a EIM-1000, it must be connected to the Gas inlet of the EIM and valves present with the sample container must be opened. Once the sample is connected to the inlet, the sample flow rate can be adjusted using the rotameter. Once gas is flowing through the EIM, the “Run”button at the bottom right of the screen in the sample (Figure 44) or calibration tab (Figure 38) will start the analysis.

The system will automatically operate the gas valve to inject the sample in the analyzer and collect analysis data. Once all the runs in a sample/standards are completed, the LUI prompts users to connect the following sample/standard (Figure 137). Users may also choose to cancel the analysis/calibration by clicking the “Cancel” button.

Figure 137

Once all samples/standards have been analyzed, the analysis is complete and the last sample/standard may be disconnected.

Section 7.4.2 – Liquid Samples Without Sample Shut Off (SSO)

Section 7.4.2.1 – General Guidelines

When using an EIM without a sample shutoff, the sample will flow freely through the entire flowpath of the EIM once the sample is loaded. Once the sample start flowing through the EIM, users must wait until no more bubbles appear through the sightglass/flowmeter. When using a flowmeter, users may adjust the flow rate to reduce sample usage. ATOM suggests a sample flowrate between 1 and 2 cc/min to ensure proper sample renewal and prevent excessive sample wasting. The flowrate on a flowmeter or sightglass EIM is adjusted by rotating the needle valve located above the flowmeter or below the sightglass. Rotating clockwise decreases flow and counterclockwise increases flow.

If bubbles do not go away, pressure sample might be too low in which case, the sample must be pressurized either by using the sample pressurizing pad feature (Section 7.4.4 – Increasing Sample Pad Pressure with EIM) or by disconnecting the sample and pressurizing it using another means.

Once the flow is properly adjusted, runs may be started and the software will automatically control the EIM and collect data from the detectors to generate a sample peak and compare to stored calibration in the case of a standard or a specific concentration in the case of a standard.

Once all runs within a samples have been analyzed, the software will prompt the user to load the next sample from the sample set. If there are no samples remaining in the sample set, the software will consider the analysis finished.

Section 7.4.2.2 – Procedure

To run a liquid sample on an EIM-1000 without a sample shut off (SSO), it must be connected to the Liquid inlet of the EIM and valves present with the sample container must be opened. Once the sample is connected to the inlet, the sample flow rate can be adjusted using the rotameter. Enough time should be given for bubbles to disappear (Section 7.4.2.2 - Procedure) or pad pressure should be applied to the sample to remove bubbles (Section 7.4.4 – Increasing Sample Pressure Pad with EIM). Once liquid is flowing through the EIM free from bubbles, the “Run” at the bottom right of the screen in the sample (Figure 44) or calibration tab (Figure 38) will start the analysis.

The system will automatically operate the liquid valve to inject the sample in the analyzer and collect analysis data. Once all the runs in a sample/standards are completed, the LUI prompts users to connect the following sample/standard (Figure 137). Users may also choose to cancel the analysis/calibration by clicking the “Cancel” button. Th

Once all samples/standards have been analyzed, the analysis is complete and the last sample/standard may be disconnected.

Section 7.4.3 – Liquid Samples With Sample Shut Off (SSO)

Section 7.4.3.1 – General Guidelines

When using an EIM with a sample shutoff, the sample will not flow through the flowpath of the EIM until the Sample Shut Off (SSO) is deactivated. Once the sample is loaded, only the path up to the SSO will contain sample.

Once the user initiates the analysis process, the software will deactivate the SSO and allow time to adjust sample flowrate through the EIM to ensure no bubbles are present in the flow path. When using a flowmeter, users may adjust the flow rate to reduce sample usage. ATOM suggests a sample flowrate between 1 and 2 cc/min to ensure proper sample renewal and prevent excessive sample wasting. The flowrate on a flowmeter or sightglass EIM is adjusted by rotating the needle valve located above the flowmeter or below the sightglass. Rotating clockwise decreases flow and counterclockwise increases flow.

If bubbles do not go away, pressure sample might be too low in which case, the sample must be pressurized either by using the sample pressurizing pad feature (Section 7.4.4 – Increasing Sample Pressure Pad with EIM) or by disconnecting the sample and pressurizing it using another means.

Once the flow is properly adjusted, runs may be started and the software will automatically control the EIM and collect data from the detectors to generate a sample peak and compare to stored calibration in the case of a standard or a specific concentration in the case of a standard.

Once all runs within a samples have been analyzed, the software will activate the SSO and prompt the user to load the next sample if other samples remain. If there are no samples remaining in the sample set, the software will consider the analysis finished.

Section 7.4.3.2 – Procedure

To run a liquid sample on an EIM-1000 with a sample shut off (SSO), it must be connected to the Liquid inlet of the EIM and valves present with the sample container must be opened. Once the sample is connected to the analyzer, only the flowpath prior to the SSO will contain sample. To adjust the flow rate, users must click the “Run” button in the sample (Figure 44) or calibration tab (Figure 38). The popup generated by the software (Figure 138) presents users with 3 choices:

Figure 138

- Purge: The SSO opens for the duration specified in the input field (*Note that this field is only editable for users with administrator or tech level access. Operators may not edit the field and the software uses the value entered in the EIM Settings tab (Section 5.6.5.3.1 – SSO Valve - Analysis Purge)*. Once the SSO is opened, sample flows through the analyzer allowing users to adjust flow and ensure that no bubbles are present. If bubbles do not disappear, pad pressure should be applied to the sample to remove bubbles (Section 7.4.4 – Increasing Sample Pressure Pad with EIM) At the end of the purge time, the SSO closes and the sample/standard is ready for analysis/calibration.

- Run: Runs the sample through the analyzer and stores peak are to generate calibration if in calibration tab or compares peak area to known calibration to calculate concentration if in sample tab.

- Abort: Abort the calibration/sample analysis

After clicking the "Run" button, the system will automatically open the SSO and operate the liquid valve to inject the sample in the analyzer and collect analysis data. Once all the runs in a sample/standards are completed, the SSO closes automatically and the LUI prompts users to connect the following sample/standard (Figure 139). Users may also choose to cancel the analysis/calibration by clicking the "Cancel" button.

Figure 139

Once all the last samples/standards has been analyzed, the analysis is complete and the sample/standard may be disconnected.

Section 7.4.4 – Increasing Sample Pad Pressure with EIM

When sample pad pressure is too low, bubbles form in the sample flowpath and take extended time to clear out. To prevent bubbles in the flowpath, sufficient pad pressure is required (ATOM recommends 200 psi for typical butane samples/standards).

The ATOM EIM-1000 allows users to apply a pad pressure on the sample using the pad pressure feature (Figure 140). To apply pad pressure to a sample, a connection hose (not provided by ATOM) is required. The hose attaches to the top of the EIM. The EIM contains a pad pressure inlet on the back. Nitrogen is used to apply pad pressure in a large number of applications (Contact the appropriate person within your organization to verify if a nitrogen pad pressure is good for your application). Once the pressure pad inlet is connected and the hose connected, users may apply pad pressure to samples using directly the EIM-1000.

To apply pad pressure, connect the hose to the sample and rotate the valve below the pad pressure gauge to the “Pad Pressure” position. The gauge directly indicates the pressure of the pad in the sample.

Figure 140 EIM-1000 with Cylinder and Hose for Pad Pressure

Section 8 – Basic Maintenance Guide

Section 8.1 – Safe Service Instructions

This section covers some basic maintenance procedures that can be performed regularly to keep the instrumentation running efficiently.
However, it is important to follow safe work measures to avoid any personal injuries and/or loss of life and/or property.
Please follow the safety guidelines in this manual very carefully. The most common maintenance tasks and the associated hazards are identified in this section. However, this manual also includes detailed information about identified risks and safe operation of the analyzer and its peripheral modules.

WARNING: **A SEVERE TO POTENTIONALLY LETHAL ELECTRIC SHOCK HAZARD MAY EXIST ON 110-240 VAC LINE COMPONENTS WHILE POWER IS APPLIED TO INTERNAL COMPONENTS.** Ensure that power is disconnected from the power source before working on the instrument.

WARNING: **HIGH-PRESSURE GASES SHOULD BE HANDLED WITH EXTREME CARE.** Ensure that all gas lines, regulators, gas purifiers, etc. are specified for the intended use. Verify that all tubing is depressurized, and sample drained before beginning work on any of the modules. Verify that lines are properly purged before opening lines or disconnecting sample.

WARNING: **EYE INJURY AND SERIOUS BURNS CAN RESULT WHEN HANDLING THE GLASS COMBUSTION TUBE.** The combustion tube is extremely hot and should not be removed from the furnace until the furnace has been allowed to cool for at least 4 hours. Wear appropriate eye protection during service, removal and replacement of the combustion tube.

WARNING: **HIGH-PRESSURE GAS BOTTLES SHOULD BE HANDLED WITH EXTREME CARE.** Typically, most sample and gas bottles are under pressures in the hundreds or thousands of PSI. Ensure that the bottle regulators are closed OFF before disconnecting lines.

CAUTION: **Recommended pressure** for combustion/carrier gas is 40 psi. The Mass Flow Controllers (MFCs) should not be operated at pressures higher than 70 PSI as it can cause fluctuations in flows and inaccurate control.

WARNING: **IMPROPER/INCORRECT TOOLS CAN CAUSE INJURY AND/OR PROPERTY DAMAGE.** Using incorrect tools can cause slippage leading to injury from loss of balance, or cuts or trauma.

WARNING: **SEVERE BURNS CAN RESULT WHEN WORKING AROUND A HOT FURNACE.** The combustion tube is extremely hot (operating temperature of 1050 °C). Allow furnace to cool down for at least 4 hours before performing any maintenance on it.

CAUTION: Carefully ensure the analytical system is free from leaks. Failure to do so may cause inconsistent analytical performance and/or system component damage.

WARNING: **COMPONENT DAMAGE MAY OCCUR WHEN USING A LIQUID LEAK DETECTOR.** Even though the solution in an approved liquid leak detector "Snoop" solution is non-conductive, care should be taken not to wet any electrical or electronic components to avoid damage to sensitive equipment. Many liquid leak detectors contain sulfur compounds that can contaminate the gas supply line and instrument flow path components. Care should be taken not to wet or contaminate the analytical flow system when using a liquid leak detector.

CAUTION: **The combustion tube inlet and outlet connections are fragile.** Care should be taken to follow the correct procedures while making these connections. Only use graphite ferrules to connect tubing to combustion tube.

CAUTION: **Do not over-tighten fittings.** Fittings should be tightened according to manufacturer's specified recommendations to prevent leaks.

CAUTION: **The Excimer UV lamp is fragile.** Care should be taken when handling and replacing it. The internal parts of the lamp consist of delicate glass.

CAUTION: **The Photo Multiplier Tube (PMT) is extremely sensitive to light.** Exposure to excessive light while PMT power is applied could result in damage to the PMT. Power to the PMT should be turned off before exposing the PMT window to any ambient light. Do not remove PMT filters while it is still powered ON.

CAUTION: **Ensure all inlet and outlet openings are kept clean and free from contaminants.** It is recommended that the inlet and outlet openings be plugged when not connected to lines.

CAUTION: **Potentially hot surfaces are identified using this warning label. Caution is required when touching hot surfaces to avoid burns and other injuries**

CAUTION:

Make sure the EIM is operated at its recommended pressure only! Exceeding the ratings can cause sample to leak under dangerously high pressures that can severe injuries and damage.

Section 8.2 – Replacing the Septum

Over time septa lose the ability to maintain leak-free seals at the XT Series Analyzer inject port and need to be replaced. The following procedure details the recommended method to replace septa and maintain seal integrity.

To release the XT Series Analyzer side panel, where the injection port is located, pull apart the two side latches as shown in *Figures 141* and *Figure 142.*

Figure 141 Opening of Side Latches

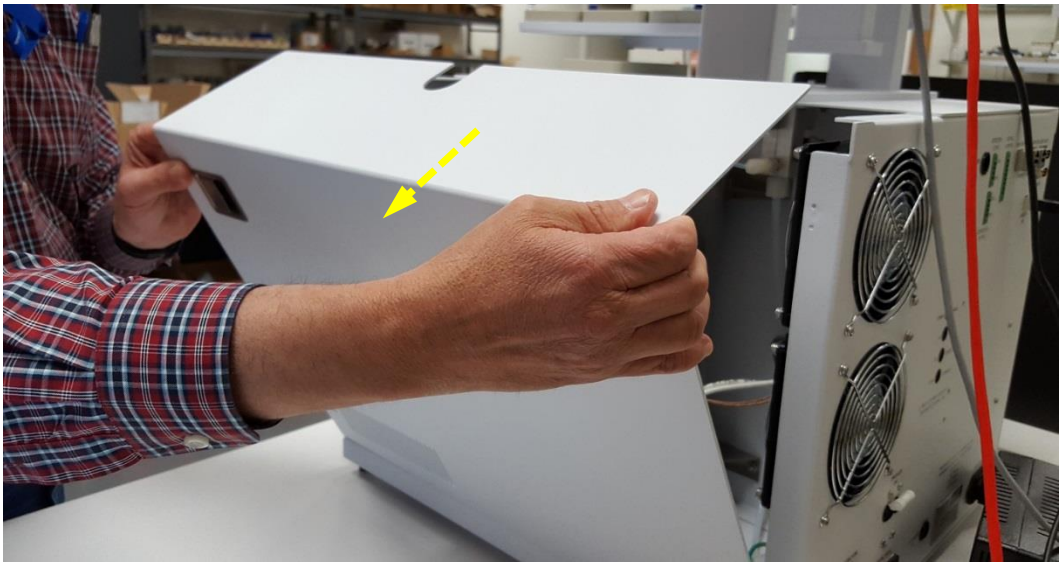


Figure 142 Removal of Side Panel

The XT Series Analyzer injection port septum is located in a septum retainer nut. Removed the nut by holding firmly the septum adapter fitting and twisting counter-clockwise the nut as shown in *Figures 143* and *144*.

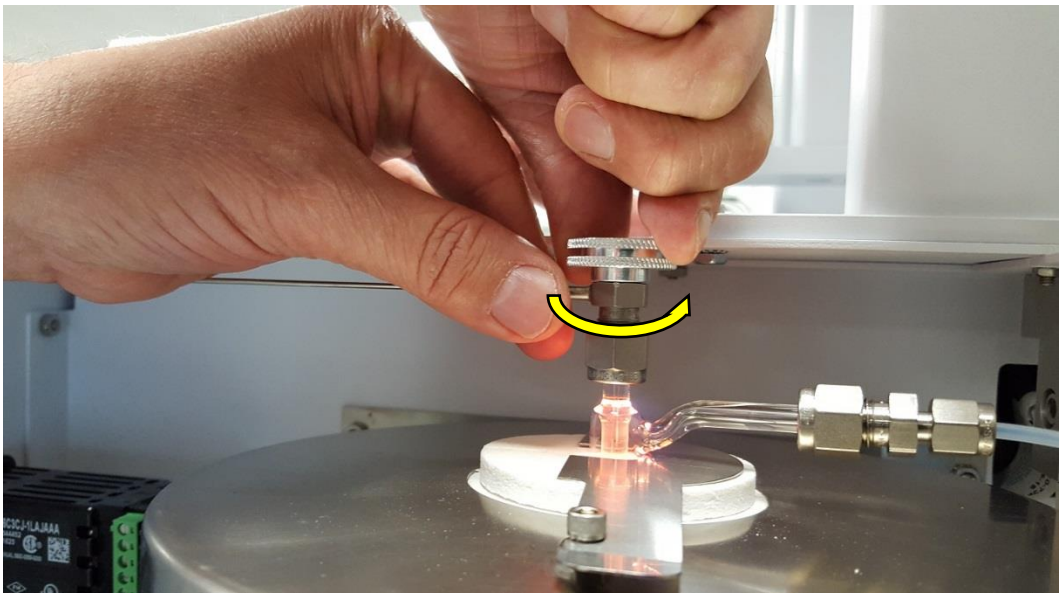


Figure 143 Removal of Septum Adapter Fitting

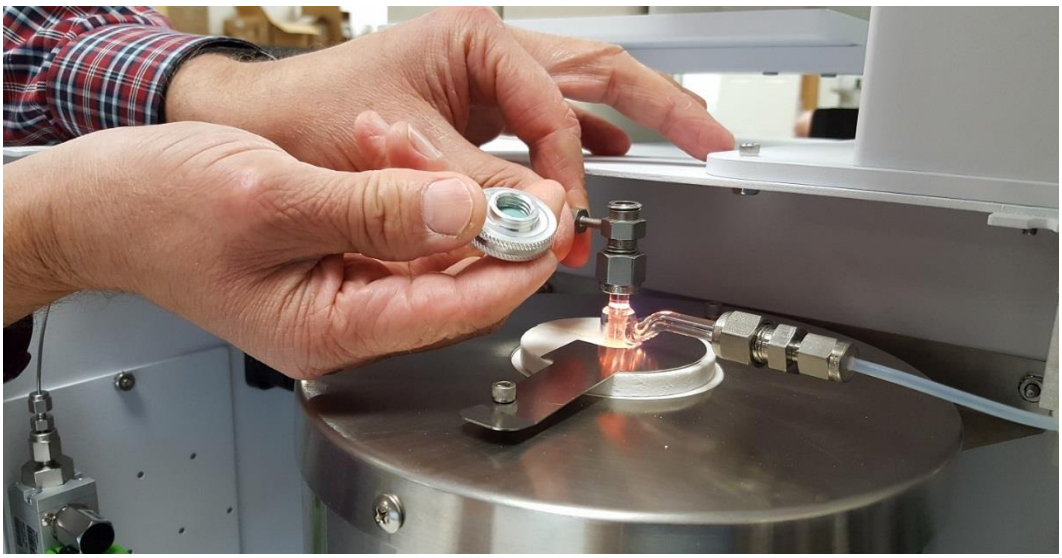


Figure 144 Septum in Septum Adapter Fitting

Push the used septum out of the retainer nut using a thin wire-tool as shown in *Figures 145* and *146.*

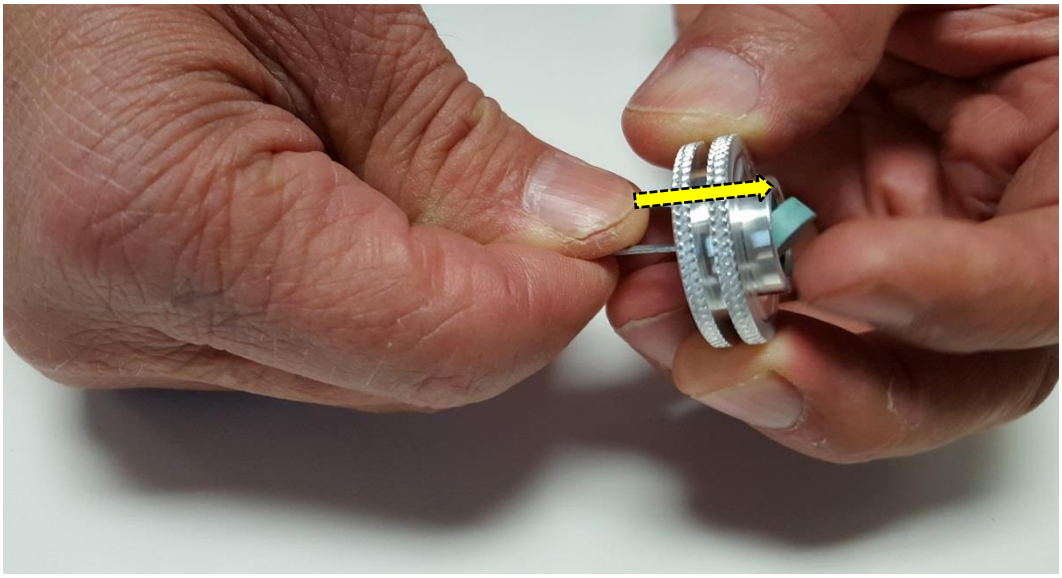


Figure 145 Removal of Used Septum from Retainer Nut

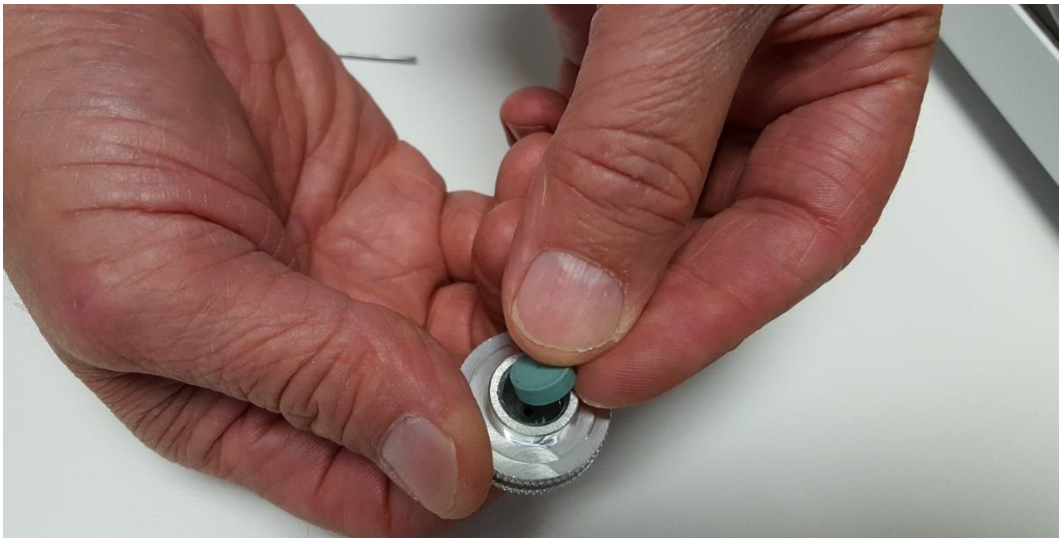


Figure 146 Used Septum out of Retainer Nut

Once the used septum has been removed from the nut, insert the new septum into the retainer nut (*Figure 147*). When inserting a new septum, take care in avoiding applying uneven pressure on the septum as it can cause deformation leading to leaks and affecting analysis results.

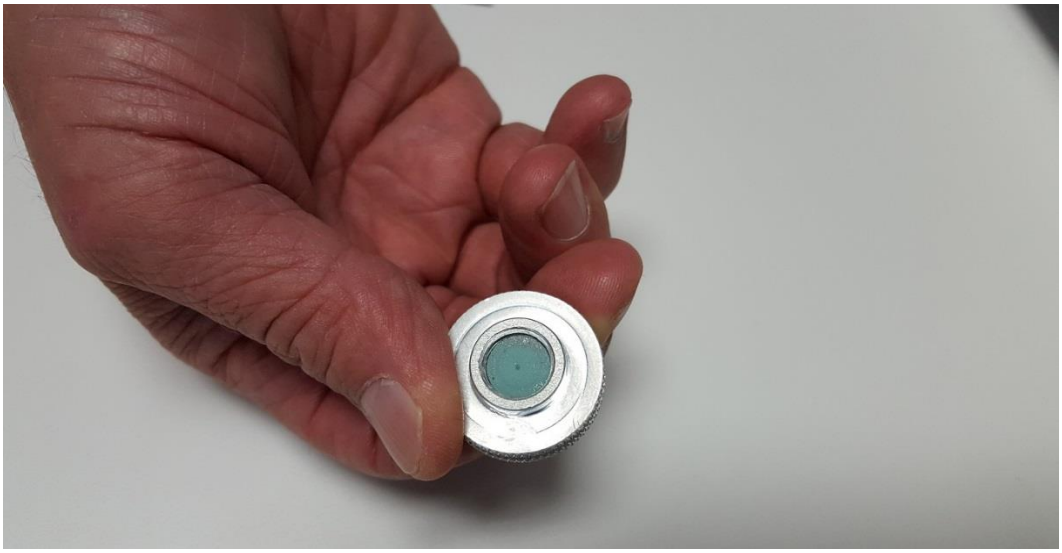


Figure 147 New Septum in Retainer Nut

To reinstall the septum retainer nut onto the XT Series Analyzer injection port, hold firmly the septum fitting adapter and twist the nut clockwise as show in *Figure 148*. *Please note that overtightening the nut may cause septum to deform.*

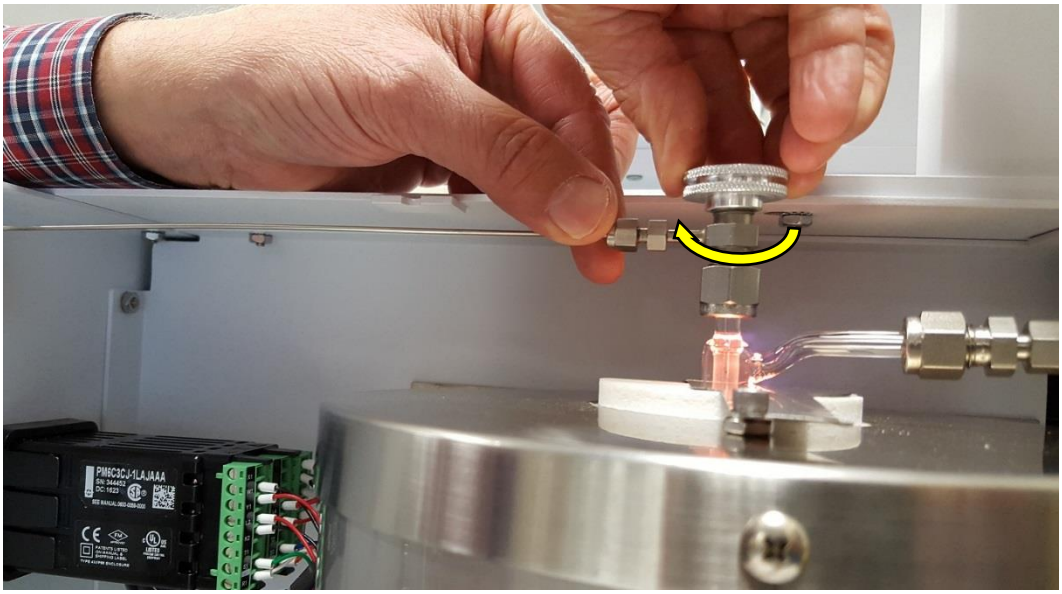


Figure 148 Reinstallation of Septum Nut onto Injection Port

Once the new septum is replace, put back and secure the side panel with the two latches as shown in *Figure 149*.

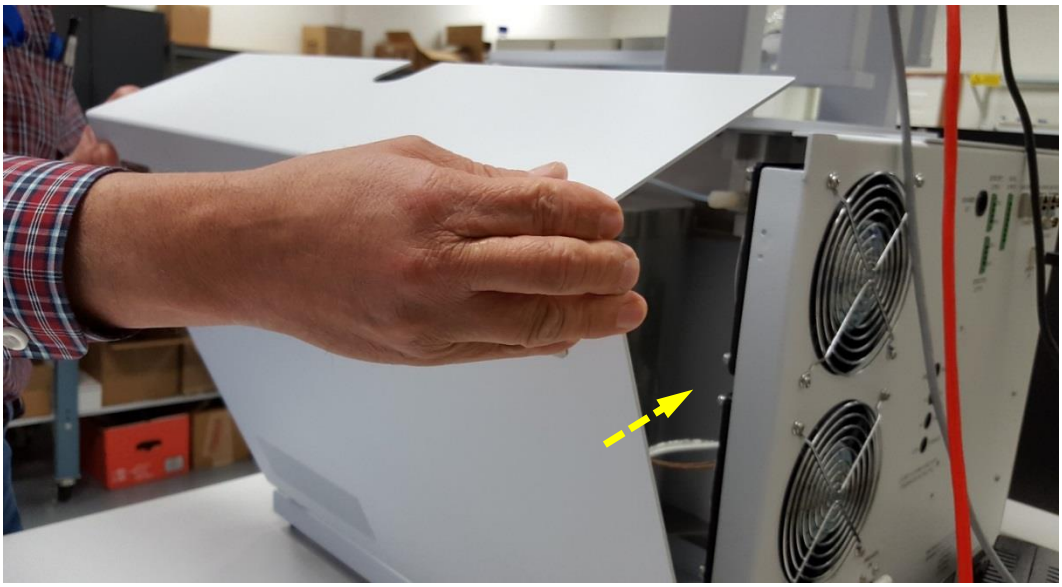


Figure 149 Reinstalling of Side Panel

Section 8.3 – Replacement of Autosampler Syringe

Autosampler syringes get damaged over time and need to be replaced. Bad syringes cause analytical errors due to the lack of repeatability in sample draw. This procedure details how to change the autosampler syringe.

Before the syringe can be physically replaced, users must access the “Service” menu to prepare the autosampler for a new syringe.

To access the Service menu on the Autosampler Input Module, access to “Extended User Level” by holding both “A” and “B” buttons on the terminal to bring up the “Change Access” screen *(Figure 150)*. Scroll down and select “Extended User Level”. An asterisk * will appear against this option indicating that the module is in Extended User Access Level (*Figure 150*).

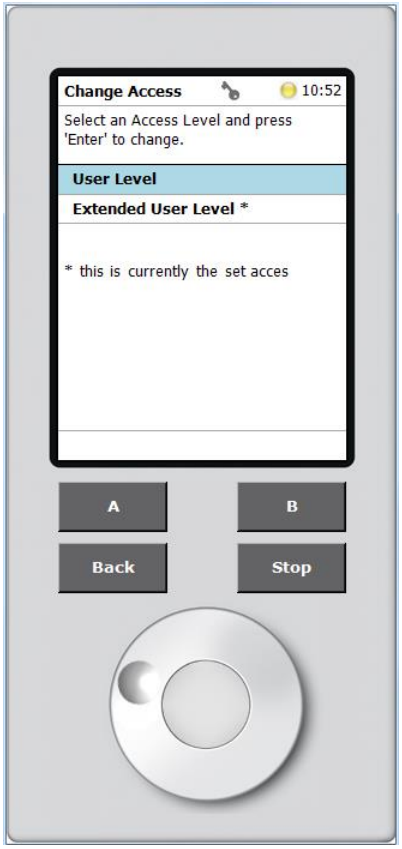


Figure 150 Extended User Level Access

Once in Extender User mode, reach the Installation menu by pressing the “A” (Options) button in the main menu, then “Service” and then “Installation” (*Figure 151*).

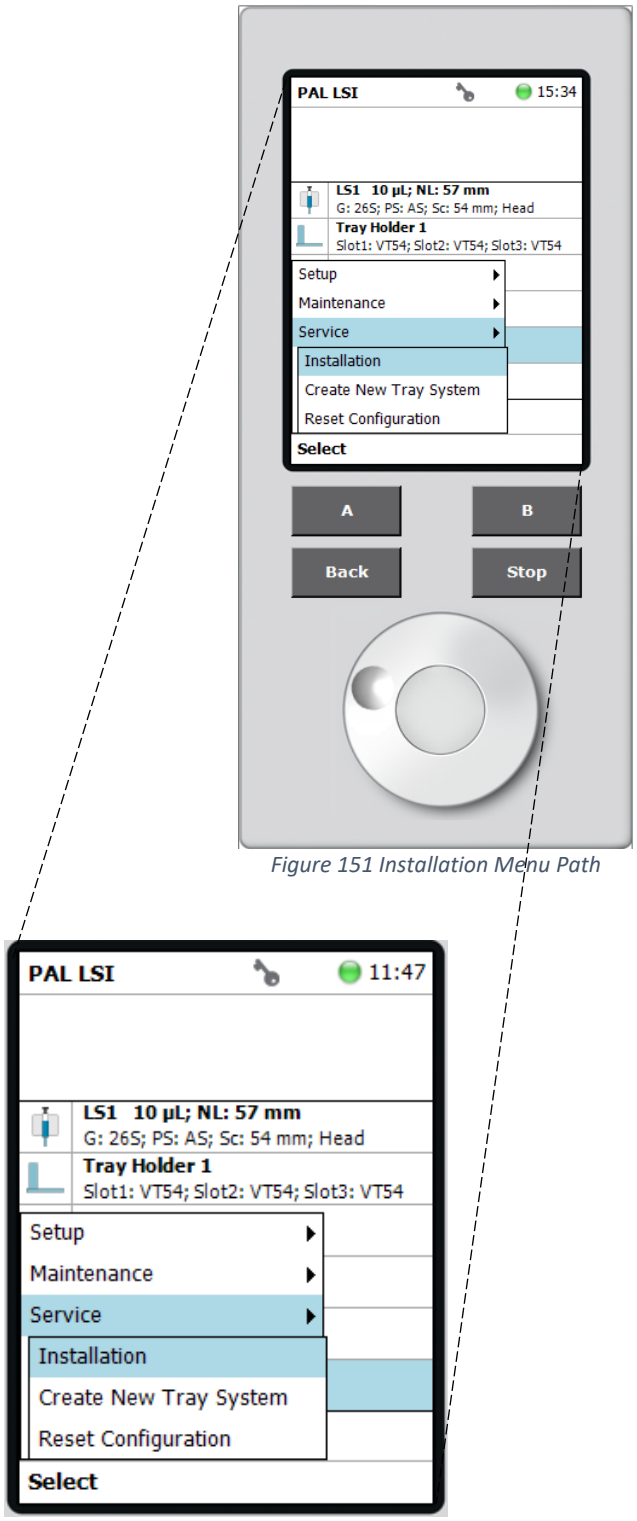


Figure 151 Installation Menu Path

In the “Installation” menu, select “Exchange Syringe” (*Figure 152*).

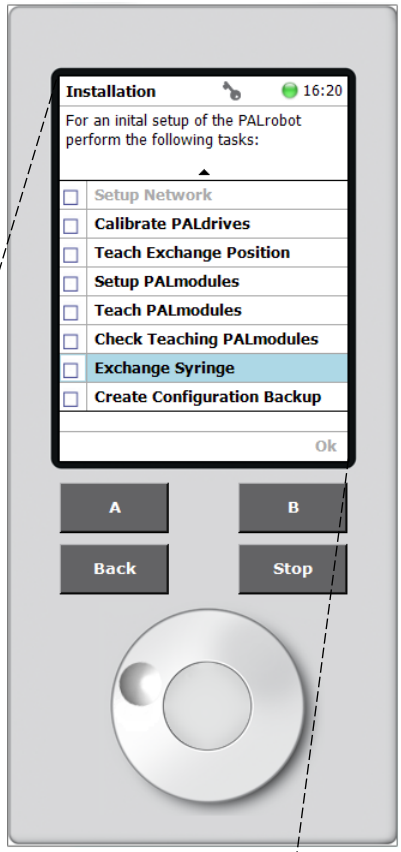
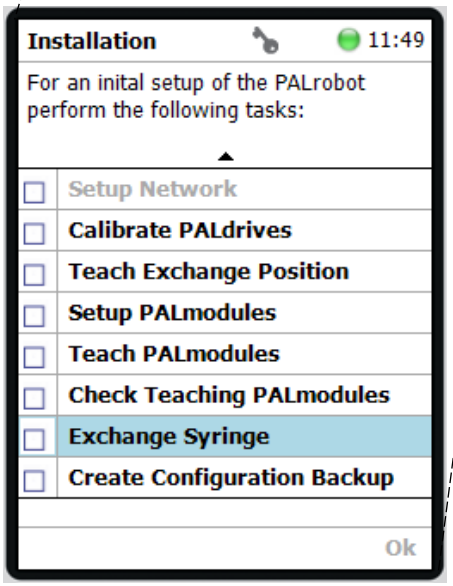


Figure 152 Exchange Syringe Option



On the following screen, press “B” (Move) for the Autosampler head to move the Injector module to the exchange position (*Figure 153*).

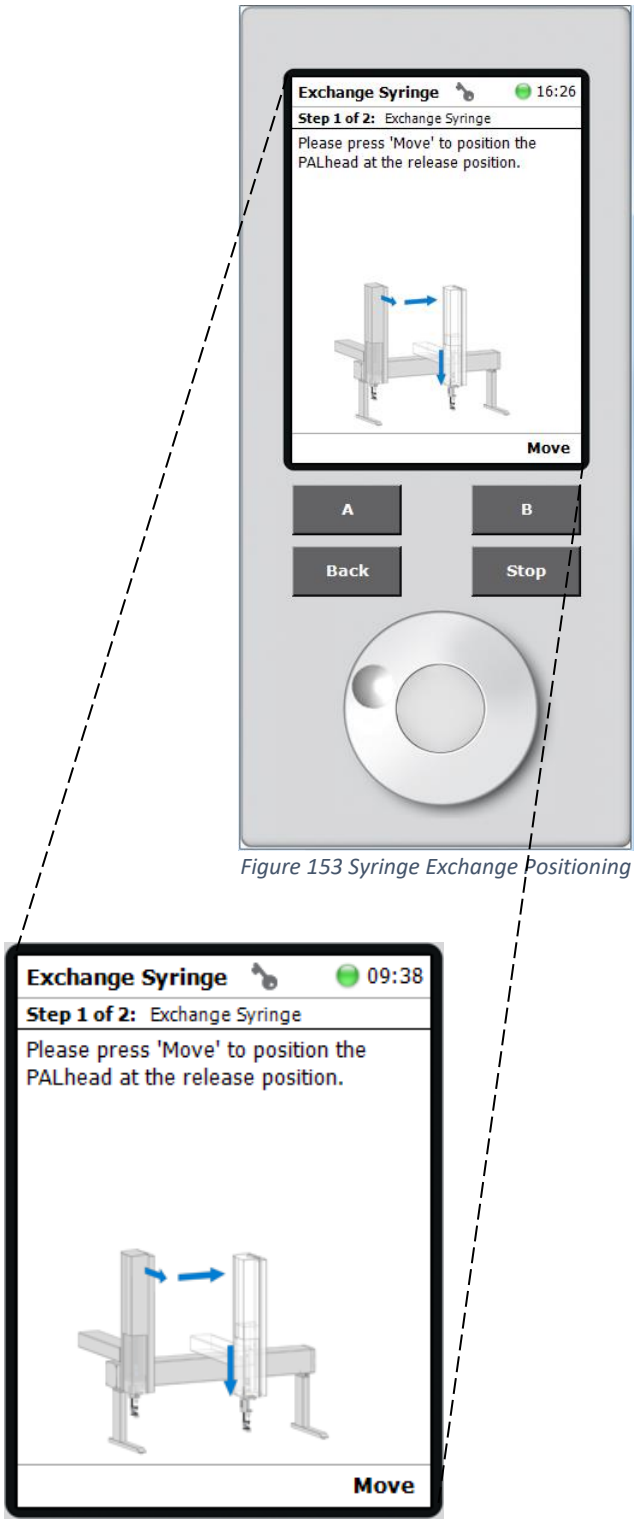


Figure 153 Syringe Exchange Positioning

The autosampler head will position itself in the exchange position with the syringe easily accessible as shown in *Figure 154*

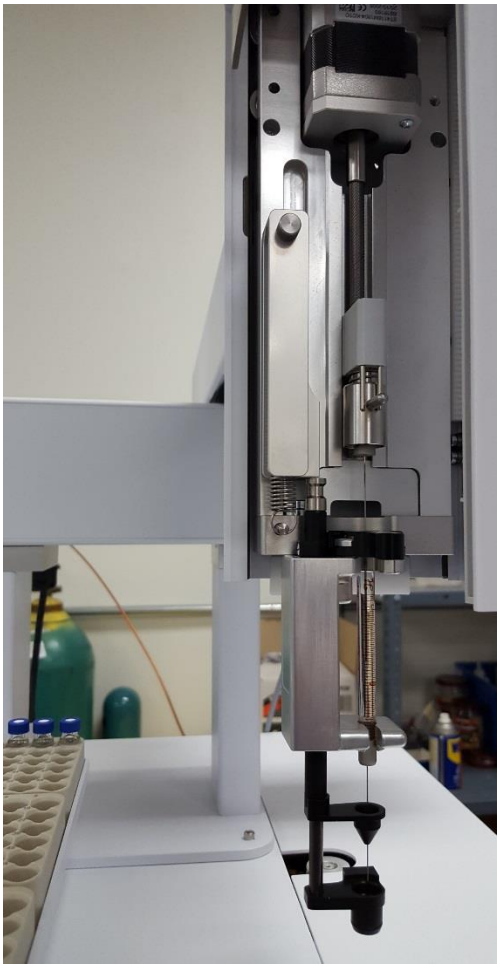


Figure 154 Autosampler Head in Exchange Position

Once in the exchange position, lift up the holding pin to bring the syringe plunger out of the syringe (*Figure 155*). To eject the syringe, pull the both the syringe plunger and holding pin apart *(Figure 156)*. *Please note that the ejector is a spring-loaded ball-bearing device and that, during release, the ejection kick forces the plunger away from the holder.*

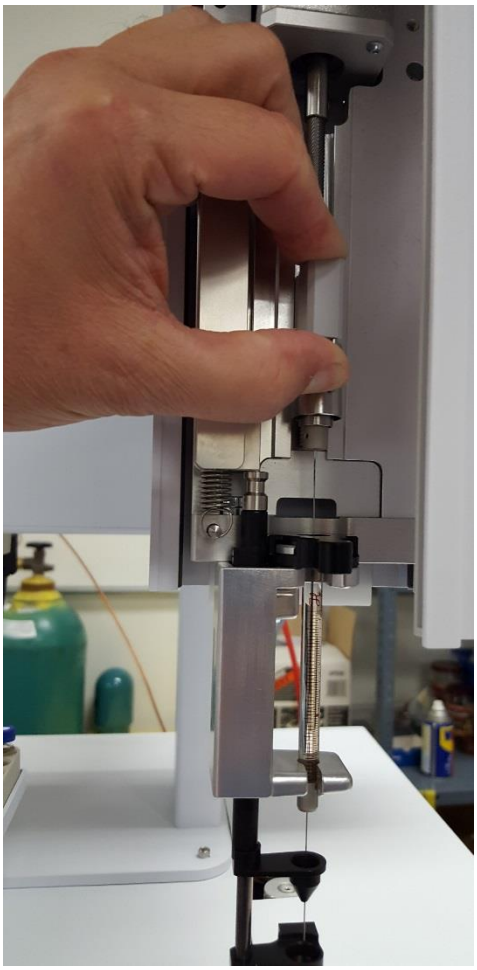


Figure 155 Extraction of Syringe Plunger

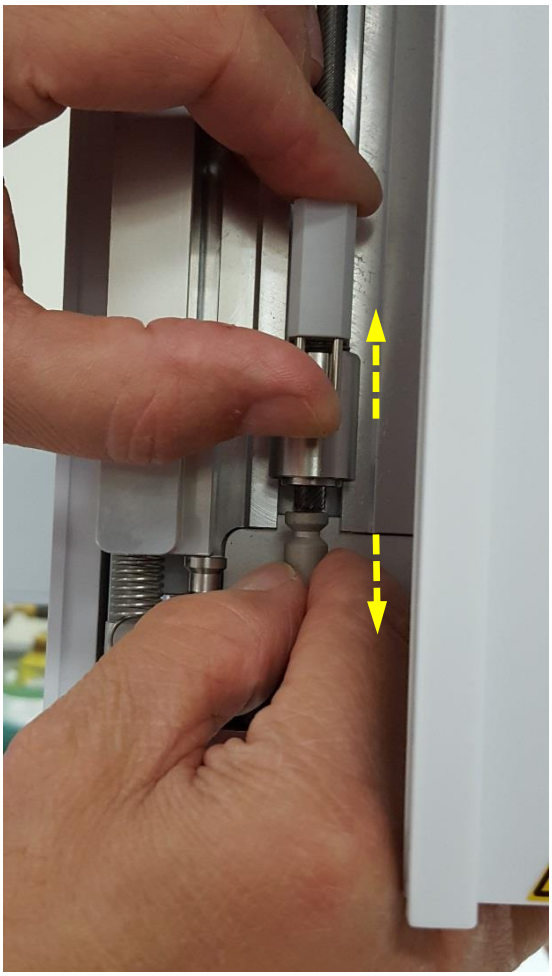


Figure 156 Release of Syringe Plunger

Once the syringe plunger is released from the holder *(Figure 157)*, push the syringe plunger all the way into the syringe *(Figure 158)*.

Figure 157 Plunger Released from Holder

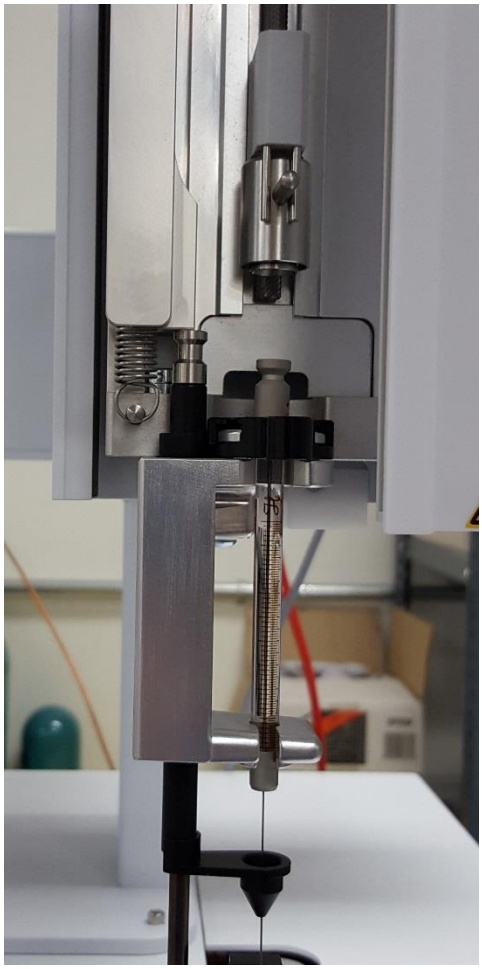


Figure 158 Plunger Pushed Entirely into Syringe

Disengage the syringe by turning the black polymer bayonet nut to the right (*Figure 159*) and lifting it out over the syringe (*Figure 160*). *Please note that bayonet nut may differ from pictures.*

Figure 159 Disengaging of Syringe

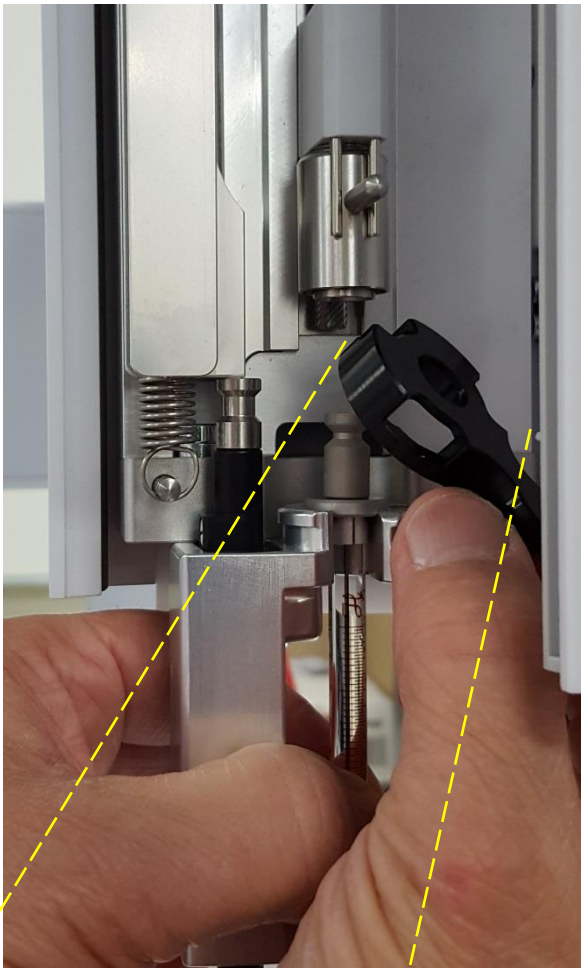


Figure 160 Removal of Black Bayonet Nut

Black Polymer Bayonet Nut

Before replacing the old syringe with a new syringe, verify where the flat edge of the new syringe is located (*Figure 161).*

Figure 161 Syringe Flat Edge

Once the bayonet nut is removed and the flat edge of the new syringe located, carefully remove the old syringe from the autosampler head *(Figure 162)*. Install the new syringe by ensuring that the flat edge faces the autosampler head and locks in position as show *Figure 163*. *Please note that if orientation is reversed, the syringe will not sit correctly in the contoured slot, and will not lock in place.*

Figure 162 Removal of Syringe

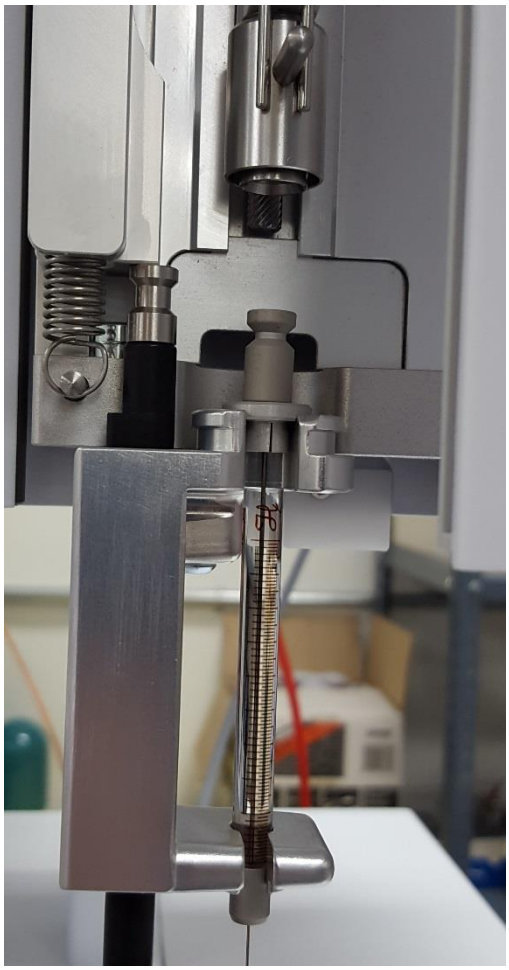


Figure 163 New Syringe Installed in Contoured Slot

To engage the new syringe, place the black polymer bayonet nut over the syringe and rotate left (*Figure 164*). To lock the syringe plunger in the autosampler head holder, push the ejector down until hearing a clicking sound (*Figure 165*).

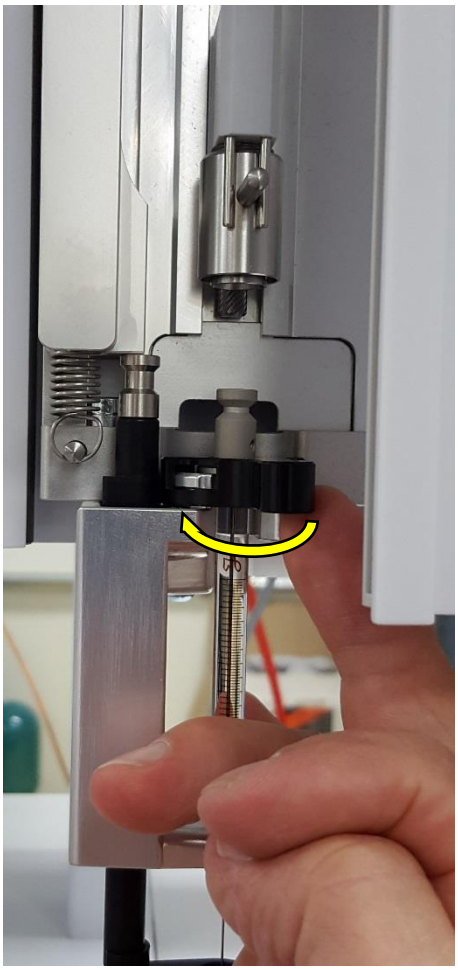


Figure 164 Syringe Engaged with Bayonet Nut

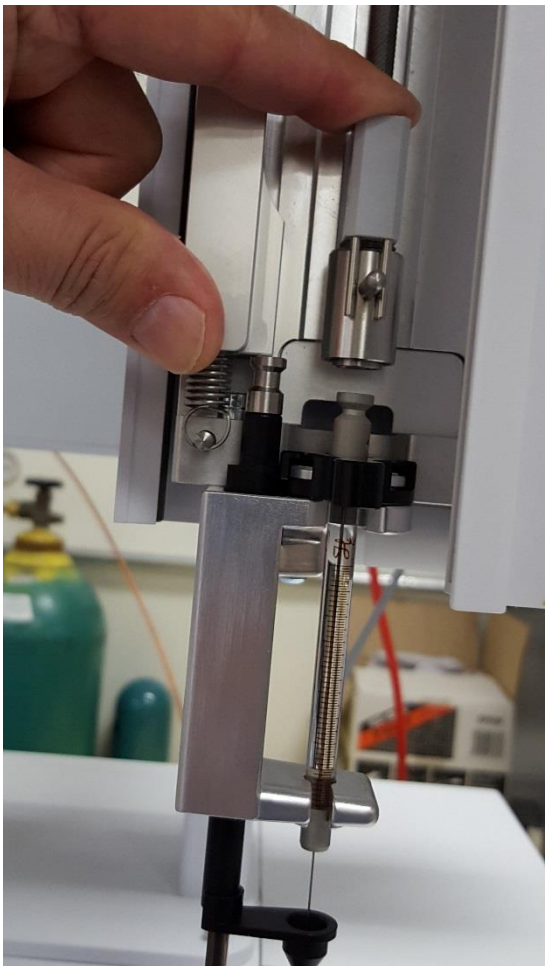


Figure 165 Locking of Syringe Plunger in Holder

Once the new syringe is installed and locked in the autosampler head, press “Next” (B button) on the autosampler terminal (*Figure 166*). When the “Exchange Syringe” screen opens showing the selected Syringe Type, verify that the correct syringe type is selected and press “OK” (*Figure 167*). By default, the ATOM syringe type is SYH207807_48mm for Air units and SYH207817_48mm for Argon/Oxygen units.

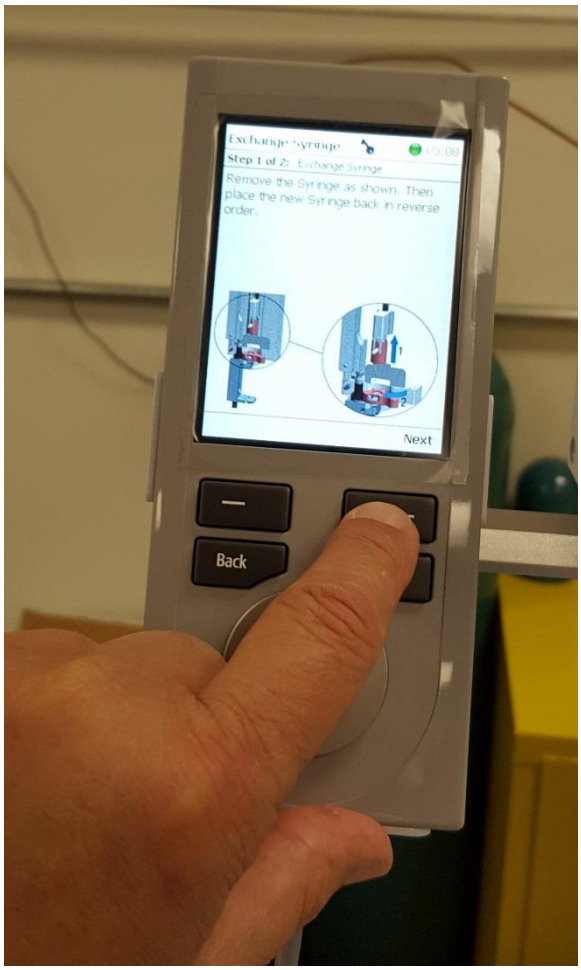


Figure 166 Completion of Syringe Exchange

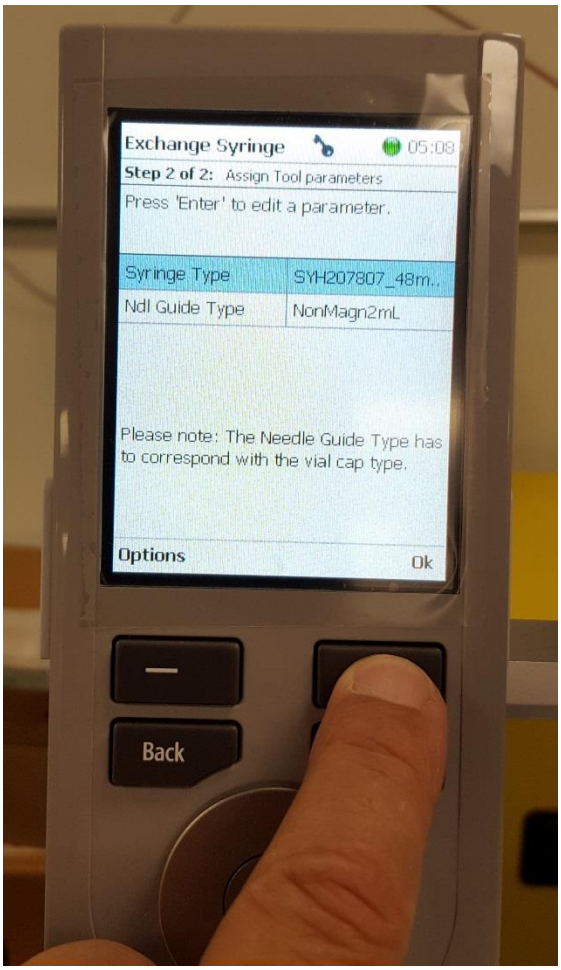


Figure 167 Selection of Syringe Type

Once the syringe type is selected, the terminal screen will revert back to the “Installation” menu. To finish the syringe exchange, press the “Back” button until you exit to the Home screen (*Figure 168*).

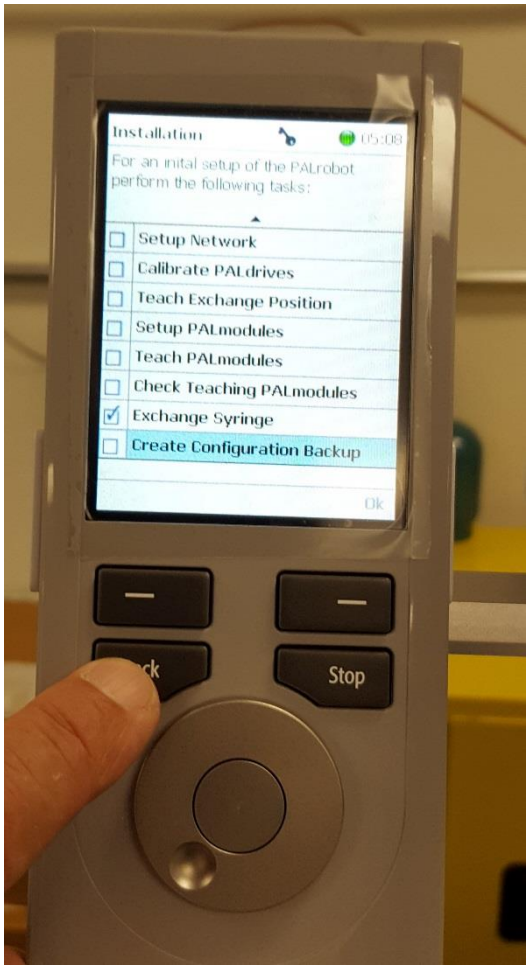


Figure 168 Return to Home Screen

Section 8.4 – Checks before returning Analyzer into service

Once the maintenance work has been completed, please perform a thorough check to verify that the system is safe to be powered up before returning the analyzer back into service.

These checks should be performed before powering up the analyzer and its peripheral modules.

- Verify that all tubings and fittings are correctly and securely connected
- Verify that all electrical connections are secure and correct
- Any gas connections should be made before turning ON the regulator
- Verify that the regulators are set at the recommended pressure
- Sample gas/liquid, if connected, should be closed OFF
- Any tools should be removed from work area
- All external devices/wires should be disconnected from the analyzer and its modules
- Make sure that the vent lines are connected and open – the detector outlet should not be blocked OFF

Once these checks are complete, the analyzer and its peripheral modules are ready to be powered ON to continue functionality testing, calibration and other software checks before returning analyzer to running samples.

Section 9 – Troubleshooting

This section covers basic troubleshooting of the XT Series analyzers, autosampler, external injection module (EIM) and LUI software. The LUI contains some built-in error reporting through pop-up error messages and the lower status bar. This section is meant to further explain some of those error messages along with problems encountered during analyzer operations not signaled with an error message.

Section 9.1 – XT Series Analyzer Troubleshooting

- *The analyzer is not starting*

  Make sure that the power outlets for both the furnace section and the electronics section are connected to a power outlet. If connected, verify that the fuse in the back of the analyzer is operational.

- *The temperature controller is blinking AL.L1*

  The temperature controller low alarm has been activated because the furnace temperature is below 1030 °C. Please verify that the furnace is powered and that the temperature settings in the LUI are set above 1030 °C.

- *The temperature controller is blinking ER.L1*

  Press the reset button on the temperature controller. If the furnace does not restart, replace the furnace thermocouple. *Please note that this error is often sign of a dying thermocouple.*

- *Upon replacing furnace thermocouple, the analyzer does not run*

  Please make sure that the thermocouple is properly inserted in the connector slots and press the reset button on the temperature controller. If still not working, please contact ATOM Instrument or your local support.

- *A Mass Flow Controller is not working*

  Verify the gas supply line and gas pressure. Mass Flow Controllers (MFC) require at least 20 psi/1.5 bar of gas pressure to operate (*Please note that ATOM Instrument recommends a gas pressure of 40 psi/ 3 bar)*. If the problem persist verify communication with CCIB board. A LED marked MFC/TC indicates if the CCIB board is communicating with the MFC.

- *Mass Flow Controllers flows are not stable and values vary excessively.*

  Make sure that the gas pressure is not too elevated and not too low. ATOM recommends keeping the gas pressure between 40 psi/3 bar and 70 psi/5 bar. If the pressure cannot be lowered within the recommended range or if multiple other systems are connected to the same gas supply line, install a pressure regulator. Alternatively, if the gas supply line is equipped with a valve (preferably ball or need), close entirely the valve and open it very slightly to allow minimum flow rate.

Section 9.2 – Autosampler Troubleshooting

- *Autosampler will not communicate with computer*

  Please verify that the autosampler is connected to the computer/network and that the proper Modbus address is entered in the LUI .config file (Section 6.5 – Communications Setup).

- *The autosampler will not let me do any modifications*

  Please verify that the autosampler is in Extended User Mode (Section 6.3 – Extended User Level).

- *The autosampler is hitting objects along travel path*

  Please verify that the autosampler path is clear from obstacles and that modules are properly taught and not only the elements (e.g.: Tray Rack and Wash Vials) contained in each module (Section 6.7 – Modules Teaching).

- *The syringe is getting damaged*

  Syringes wear out over time. If the needle is damaged, make sure the elements of each module are properly taught (Section 6.7 – Modules Teaching) and that the bayonet nut is installed on the syringe (Section 8.2 – Replacement of Autosampler Syringe).

- *The autosampler is not injecting after going through the first steps on the analysis cycle*

  Verify the autosampler parameters in the Autosampler Settings Tab (Section 5.6.4 – Autosampler Settings Tab).

- *The autosampler is aborting abruptly*

  If the autosampler starts the analysis process and aborts abruptly, verify that the various modules are present and defined (Section 6.6 – PALModules Setup).

Section 9.3 – External Injection Module Troubleshooting

- *The EIM is not responsive*

  Make sure the EIM is properly powered and that the power is on. Red lights inside the EIM indicate that the power is on.

- *Bubbles in LPG sample do not go away*

  LPG are gases at ambient pressure and temperature. When the EIM is first loaded with sample, bubbles will appear in the flowmeter/sightglass until the flowpath is filled with LPG. When the sample pressure is too low, bubbles start to appear as the LPG evaporates. To prevent bubbles from forming in the sample, ensure there is sufficient pad pressure on the sample. ATOM

recommends a 200 psi (14 bar) pad pressure for butane LPG. The pad pressure may be applied directly using the EIM. (Section 7.4.4 – Increasing Sample Pad Pressure with EIM)

- *There is no peak after sample is injected*

  Verify that the sample is properly connected to the EIM and that any valve or locking mechanism is open to allow proper flow rate. If sample is flowing through the EIM, make sure that there is sufficient carrier flow coming out of the EIM ("To Analyzer" port on the lower left side of the back of the EIM). If no flow is coming out of the EIM, verify that carrier flow is reaching the MFC and that the transfer line from the Liquid/LPG valve is not plugged/damaged.

- *Injected sample appears on the following analysis cycle*

  When injecting a sample with the EIM, the sample is carried from the EIM to the analyzer. The Mass Flow Controller inside the EIM controls the injection speed of the sample. If the EIM setpoint is too low, the sample will not reach the analyzer in time before the analysis is finished. Default EIM settings value are **12 cc/min for Air** only analyzers and **25 cc/min for Argon/Oxygen** analyzers. **WARNING:** If the EIM Mass Flow Controller Set Point is too elevated, the analyzer will coke. Increasing MFC set point should be one in increments of 1 cc/min.

- *The analysis results in long tailing peaks*

  Make sure that the heated transfer line is properly connected to the power supply and that enough time has elapsed (at least 15 minutes) to allow for the transfer line to reach operating temperature

Section 9.4 – LUI Troubleshooting

- *Analyzer goes into Idle Mode and "Red" status after running samples*

  Verify Idle Mode settings (Section 5.5.1 – Automatic Idle Mode Settings).

- *In the instrument tab, the CCIB board communication button is red*

  Verify that the USB cable between the computer and analyzer is installed. On the CCIB board inside the electronics side of the analyzer verify that the CCIB Board is communicating with computer by locating the LED called PC. If the LED is off, verify in the computer Device Manager that the allocated computer COM ports are labelled COM 5, COM 6, COM 7 and COM 8. If COM ports have the appropriate names, restart XT Service in the computer Services settings.

- *When running a sample/calibration, the peak is off scale*

  Modify PMT settings (Section 5.6.2 – Detector Settings Tab) to have a peak height below 65 million counts.

- *Drifting baseline*

Please make sure the analytical path is clear of contaminants and that the analyzer environment is stable.

- *There is no output from detector and/or UV lamp*

  Please verify that the UV lamp and or detector are turned on (Section 5.6.2 – Detector Settings Tab).

- *Concentration displays "Infinity" when doing an analysis*

  Please make sure that a density is inputted in the appropriate slot (Section 5.6.8.1.3 – Calibration Settings or Section 5.7.4 – Sample Settings).

- *Concentration displays "0" when doing an analysis*

  Please make sure that the dilution inputted factor inputted is appropriate: 1 for no dilution, a value between 0…1 depending on the dilution (Section 5.6.8.1.3 – Calibration Settings or Section 5.7.4 – Sample Settings). If running a sample, ensure that the dilution factor is greater than 0 (Section 5.7.4 – Sample Settings)

- *I cannot select a specific method to run a sample*

  Make sure the desired method is calibrated as it will not appear in the available methods list for sample analysis until it is calibrated (Section 5.6.8 – Calibration Tab)

- *There is a lot of variation in peak shape from analysis to analysis*

  Please make sure that the sample is not changing (reacting, evaporating, solidifying, etc…) between analysis. If using an autosampler, consider changing the septum and/or syringe (Section 8).

Section 10 – Certification

Certificate of Conformance

European Community Council Directive 2014/35/EC

Issue Date: 28 April 2022

COSA Xentaur Corporation hereby acknowledges that the Laboratory – Test Equipment XT-2000 and EIM-1000 has been designed and is in conformity to the following standards:

EN61010-1:2010 – 3rd Edition

EN61326-1:2013 Group 1, Class A

CISPR 11:2009 Radiated Emissions

CISPR 11:2009 Conducted Emissions

EN 61000-4-2:2008 Electro-Static Discharge Immunity

EN 61000-4-3:2006+A1+A2 Radiated, Radio-Frequency, Electromagnetic Immunity

EN 61000-4-4:2004+A1 Electrical Fast Transient/Burst Immunity

EN 61000-4-5:2005 Immunity to Surges

EN 61000-4-6:2008 Conducted, Radio-Frequency, Electromagnetic Immunity

EN 61000-4-8:2009 Power Frequency Magnetic Field Immunity

EN 61000-4-11:2004 Voltage Dips/Interruptions Immunity

The authorized signatory to this declaration, on behalf of the manufacturer is identified below:

Scott Fleishner

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Group President, Industrial & Technical Services Cosa Xentaur Corporation
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