White Paper

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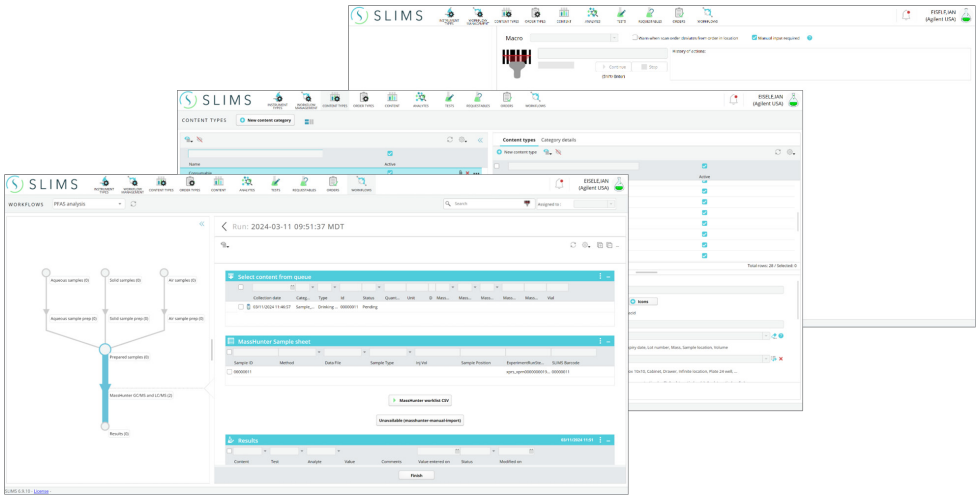
Centralizing the Management of PFAS Testing with Agilent SLIMS



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Introduction

Per- and polyfluoroalkyl substances (PFAS) are a group of synthetic chemicals used extensively in consumer products and industries due to their unique and useful properties. However, their widespread and persistent presence in the environment has raised concerns and made monitoring them a top priority for environmental testing laboratories. The recent implementation of new PFAS standards, including the United States Environmental Protection Agency (US EPA) method 1633, presents significant challenges for laboratories. These challenges include the need for sensitive instrumentation capable of detecting low concentrations, stringent contamination prevention measures, and robust data management systems to ensure regulatory compliance and data integrity.[1]

Agilent provides innovative solutions to tackle the challenges of analyzing these substances. These solutions include PFAS-free consumables, sample preparation tools to extract PFAS from complex samples, and ultrahigh-performance mass spectrometers for their analysis. To effectively manage lab efficiency, data integrity, and regulatory compliance, a digital lab transformation is crucial. Agilent SLIMS plays a pivotal role in this transformation, centralizing functions such as sample tracking, inventory management, sample preparation, and reporting into a unified platform. SLIMS offers a single interface to oversee the entire sample journey, from sample reception to regulatory reporting, making it an indispensable tool for laboratories seeking efficiency and accuracy.

Agilent SLIMS overview

Agilent SLIMS is a comprehensive solution that merges the capabilities of a Laboratory Information Management System (LIMS) and an Electronic Laboratory Notebook (ELN) into a Laboratory Execution System (LES). SLIMS is designed with convenience and flexibility in mind. It requires no client-side software and can be accessed via a Web browser from any client, including a tablet. It can be tailored to meet the specific needs of any laboratory, ensuring a perfect fit with existing workflows and processes. This extensibility expands to integration with other systems, such as existing LIMS, pH meters, balances, and instruments, ensuring seamless operation within the lab's ecosystem. Agilent can host SLIMS on a scalable, secure server, or it can be hosted on a preferred cloud service provider. Alternatively, it can be installed on-premises within your IT infrastructure, providing full control over your data and security.

SLIMS can be deployed and operational in just a few days thanks to the wealth of prebuilt configurations. One such example is SLIMS for PFAS. This package includes ready-made content such as PFAS-specific consumables, ready-to-use sample preparation protocols, and preconfigured regulatory limits for EPA methods 533, 537.1, 1633, and 8327. The capabilities included in SLIMS for PFAS can get your PFAS workflows up and running within days while also supporting tailor-made configurations to fit your evolving operating procedures. The journey through the SLIMS-enabled lab is illustrated in Figure 1 and detailed in this document.

Order intake

For many labs, sample logging, chain of custody, and order management are a major pain-points—often requiring multiple forms to be signed and data to be entered in sample tracking logbooks, spreadsheets, or legacy LIMS systems. With SLIMS, you can take the pain out of taking custody of a sample. Agilent SLIMS allows you to track the complete order life cycle from requested analyses to the validated results. The SLIMS Orders module allows anyone in your lab or in the field to quickly generate an order, enter sample and sampling container details, print a barcode label, and easily track the real-time status of the sample in-transit (Figure 2). Once the sample arrives in the lab, SLIMS makes it simple to sign for chain of custody. Routing of the samples and assignment to personnel can all take place within SLIMS. Users can be assigned requests for testing directly from the order management module, and the users can be configured to have access to exactly what they need to complete their tasks.

Figure 1. PFAS workflow overview for SLIMS. MassHunter is involved in the Analysis and Reporting sections.

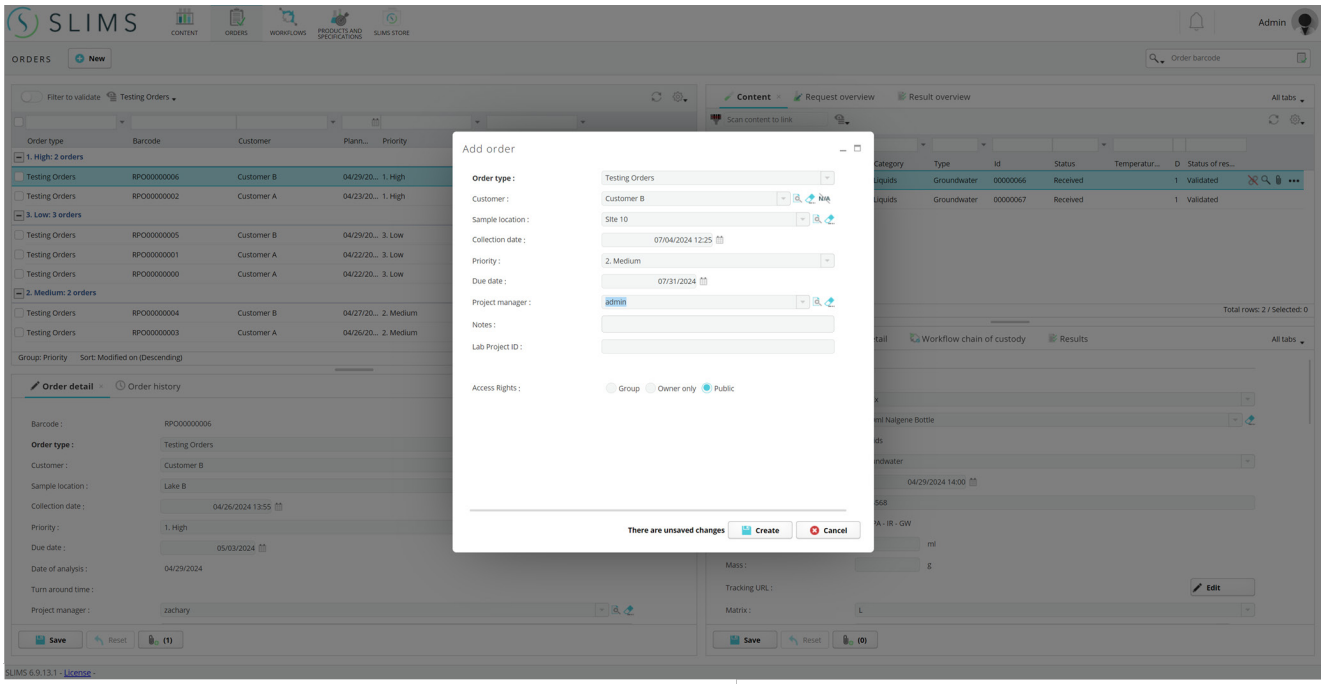


Figure 2. New order creation within the SLIMS orders module.

Inventory management and analytical requests

Accurate tracking of information such as expiration dates, inventory levels, consumable part numbers, and lot numbers is essential in a laboratory setting. Without a centralized, purpose-built system like Agilent SLIMS, these data points must be manually tracked across disparate systems, including paper records, leading to inefficiencies and increased risk of error. Agilent SLIMS improves laboratory operations by managing all laboratory content and context, enhancing productivity, and ensuring accuracy.

In SLIMS, every item in a laboratory's inventory—including trays, sample vials, consumables, columns, and solvents—is categorized as a 'content type' (Figure 3). This categorization enables the system to associate specific details with each item, such as quantities, expiration dates, and storage locations. For instance, consider the Agilent Bond Elut PFAS WAX cartridge, a PFAS-specific consumable, preloaded with the PFAS package. SLIMS provides a comprehensive view of all information linked to this cartridge. The content concept centralizes access to valuable data such as part number, lot number, location, quantity, and even a hyperlink for online reordering. This cartridge, or content, is also linked to the preconfigured PFAS sample preparation protocols, which will be discussed in more detail later. When a SLIMS user runs a sample preparation protocol, any consumables or other items used in the process are recorded and their inventory is updated. This system facilitates complete traceability of not only sample information, but all items, procedures, instruments, and personnel involved in the processing of the sample.

SLIMS makes it simple to pre-define tests, analytes, and specifications for analytical tests that are ordered. Also, the graphical path through a workflow can also be predefined so that the right sample prep and analysis protocols are automatically chosen for the user preventing guesswork, limiting operator error. The analytical requests ensure that your samples are always routed correctly through the most complex workflows.

Automation and customization are key to user-friendly workflows and simplified record keeping. SLIMS enables users to replace many of the manual actions performed within the software with automated macros. Macros are no-code, sequences of steps that streamline repetitive tasks, ensuring consistency and saving valuable time. Figure 4 shows an example of one such macro, to automate the creation of a new consumable, which automates the addition of a solution of 0.1M formic acid to the lab's stock room inventory, including any necessary record keeping steps. Macros are user created, can be used in many places throughout SLIMS, and are another tool for tailoring SLIMS to the specific needs of a lab.

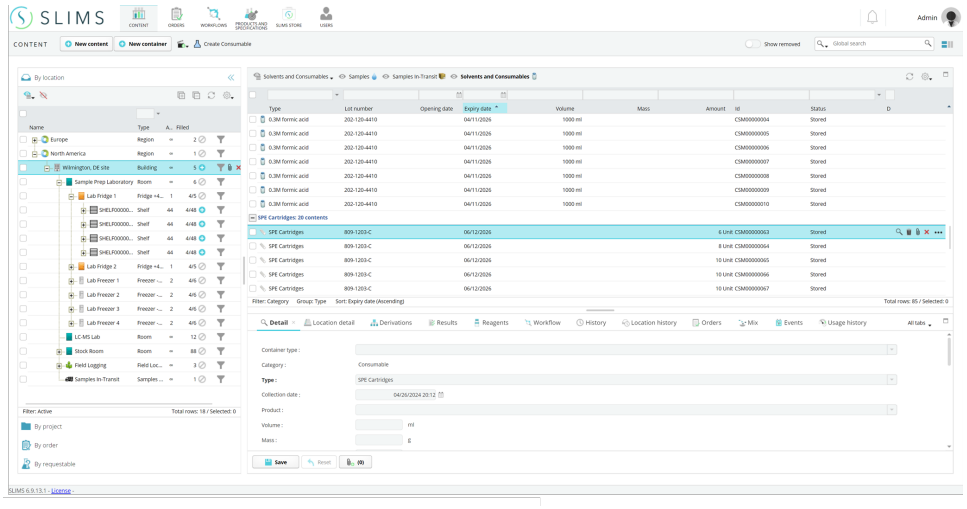


Figure 3. Location hierarchy and details within the SLIMS Content module.

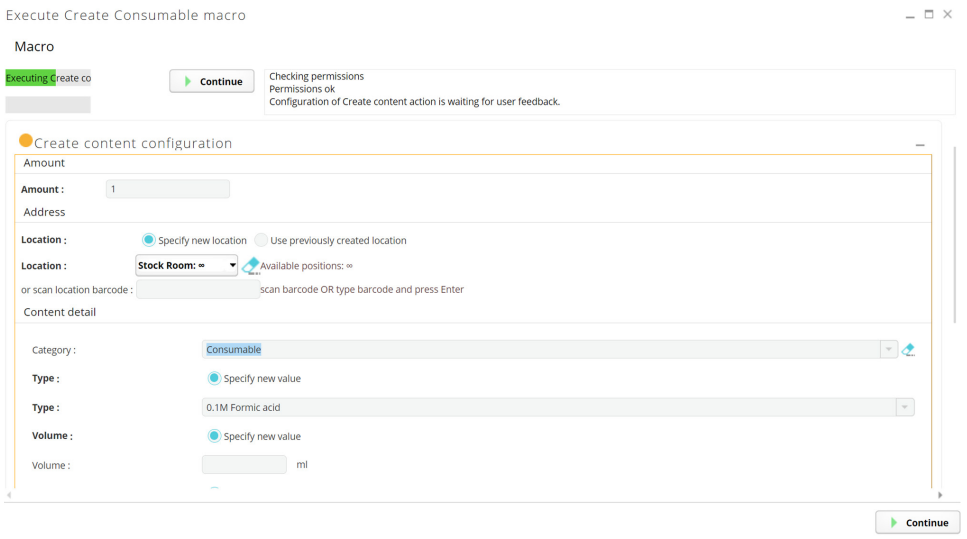


Figure 4. Customizable macro to automate the creation of new content within SLIMS.

Sample preparation

Protocols are a core function within the SLIMS Workflows module, ensuring laboratories follow established guidelines, reduce errors, and improve results. SLIMS guides users through predefined protocol steps for sample preparation and other tasks, recording all necessary procedures, measurements, and notes for complete traceability (Figure 5). The PFAS package includes specific protocols for both aqueous samples (wastewater, surface water, groundwater, and landfill leachate) and solid samples (soil, sediment, and biosolids) based on U.S. EPA Method 1633 and Agilent application notes[1,2,3].The protocols are enhanced with macros and other customized scripts to automate many tasks a user must perform. For example, when an SPE (solid phase extraction) cartridge is used in a sample preparation protocol, the inventory level is automatically updated, and the lot number is recorded with the sample.

Analysis and reporting

After the sample preparation protocols are completed, the PFAS protocol guides the user to create a sample sheet, commonly referred to as a worklist, for use in MassHunter software. EPA 1633 contains specific requirements for the batch of samples, including instrument blanks and quality controls, combined with 10 or fewer samples at a time. SLIMS programmatically builds this sample sheet from the samples currently in process within the current run of the PFAS workflow (Figures 6 and 7). The user then exports the sample sheet from SLIMS as a CSV (comma-separated values) file, properly formatted to be imported as a MassHunter worklist (Figure 8).

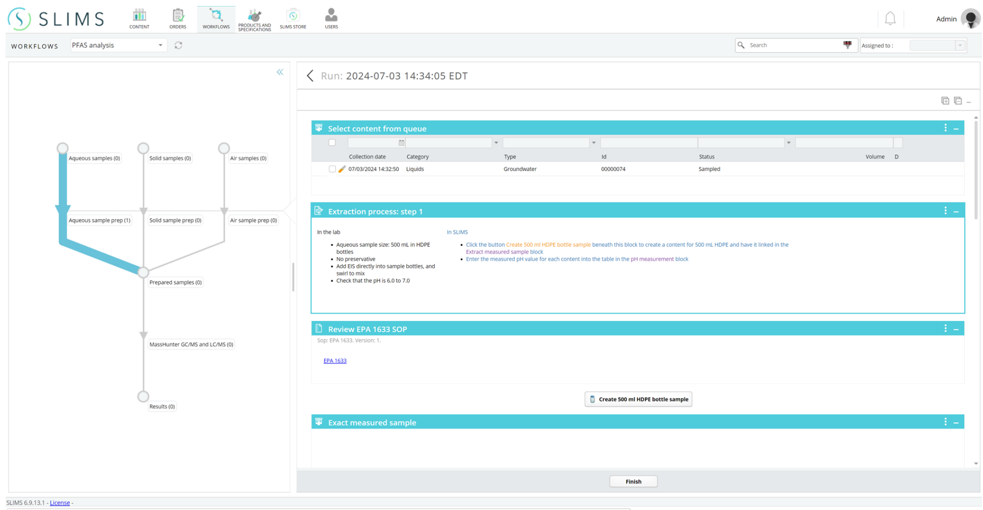


Figure 5. SLIMS protocol for the preparation of PFAS samples for analysis.

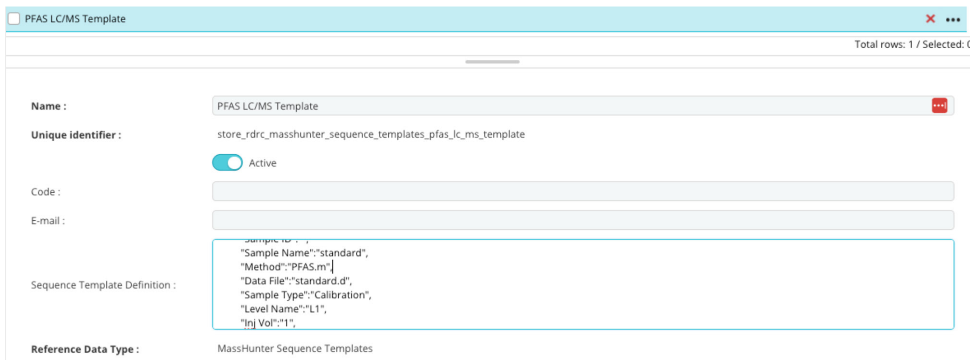


Figure 6. Automation script within SLIMS for the generation of the EPA 1633 sample batch.

MassHunter Sample sheet

Sample ID	Sam...	Met...	Data...	Sam...	Level...	Inj Vol	Sam...	Dilut...	Wt/Vol	Com...	User...	User...	User D...
00000114		PFAS.m		Sample		1		1	2		00000114	xrsc_xpr...	xprs_xprn...
BLNK00000010		PFAS.m		Sample		1		1	2		BLNK00...	xrsc_xpr...	xprs_xprn...
PFAS00000009		PFAS.m		Sample		1		1	2		PFAS00...	xrsc_xpr...	xprs_xprn...

Figure 7. MassHunter sample sheet generated in SLIMS.

Sample ID	Sample Name	Method	Data file	Sample Type	Level Name	Inj Vol	Sample Posit	Dilution	Wt/Vol	Comment	User Defined 1	User Defined 2
	standard	PFAS.m		Calibration	L1	1						xprs_xprn0000000027_store_xptm_pfas_analysis_
	standard	PFAS.m		Calibration	L1	1						xprs_xprn0000000027_store_xptm_pfas_analysis_
	standard	PFAS.m		Calibration	L1	1						xprs_xprn0000000027_store_xptm_pfas_analysis_
	standard	PFAS.m		Calibration	L1	1						xprs_xprn0000000027_store_xptm_pfas_analysis_
	standard	PFAS.m		Calibration	L1	1						xprs_xprn0000000027_store_xptm_pfas_analysis_
	standard	PFAS.m		Calibration	L1	1						xprs_xprn0000000027_store_xptm_pfas_analysis_
PFAS00000107		PFAS.m		Sample		1		1	2		PFAS00000107	xprs_xprn0000000027_store_xptm_pfas_analysis_
PFAS00000008		PFAS.m		Sample		1		1	2		PFAS00000008	xprs_xprn0000000027_store_xptm_pfas_analysis_
	blank	PFAS.m		Blank		1						xprs_xprn0000000027_store_xptm_pfas_analysis_
	blank	PFAS.m		Blank		1						xprs_xprn0000000027_store_xptm_pfas_analysis_

Figure 8. CSV file export of the MassHunter sample sheet generated in SLIMS.

Running the worklist in MassHunter is streamlined using MassHunter Study Manager (Figure 9). Study Manager is a tool included with MassHunter that lets you create a queue of analyses, or studies, to run sequentially. A study is a collection of samples and operations that are grouped together and contain the necessary information to automate the injection, acquisition, and data analysis of each sample. The CSV sample sheet generated during the SLIMS PFAS MassHunter protocol contains fields such as sample name, acquisition method name, quant method name, and LIMS IDs. Other information such as study folder path are set up in Study Manager.

Once the analysis of each study is complete, the results are calculated and reported using MassHunter Quantitative Analysis. The option to generate an XML (Extensible Markup Language) results file is selected in MassHunter and is used to transmit the results to SLIMS. A PDF (Portable Document Format, Figure 10) template for EPA 1633 is available through Agilent SubscribeNet and can be uploaded and attached as a record in SLIMS, linked to the appropriate content. Both files are saved to a network shared folder, which SLIMS will monitor for new files. Once the results are uploaded to SLIMS, the values can be evaluated against predetermined specifications included with the PFAS package. These evaluated results, along with all other data relevant to an analysis, can then be used to generate a certificate of analysis and are available for further digital reporting (Figure 11).

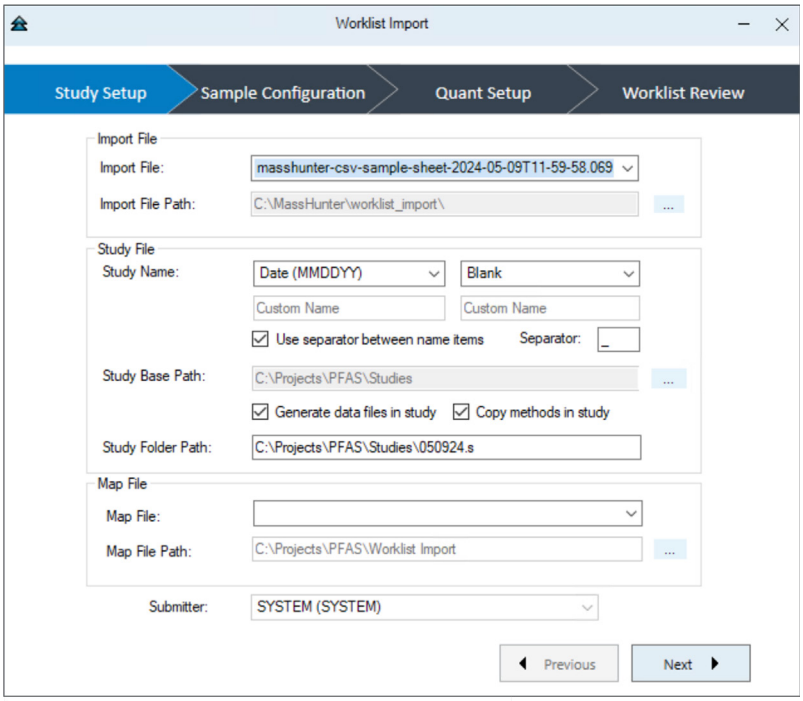
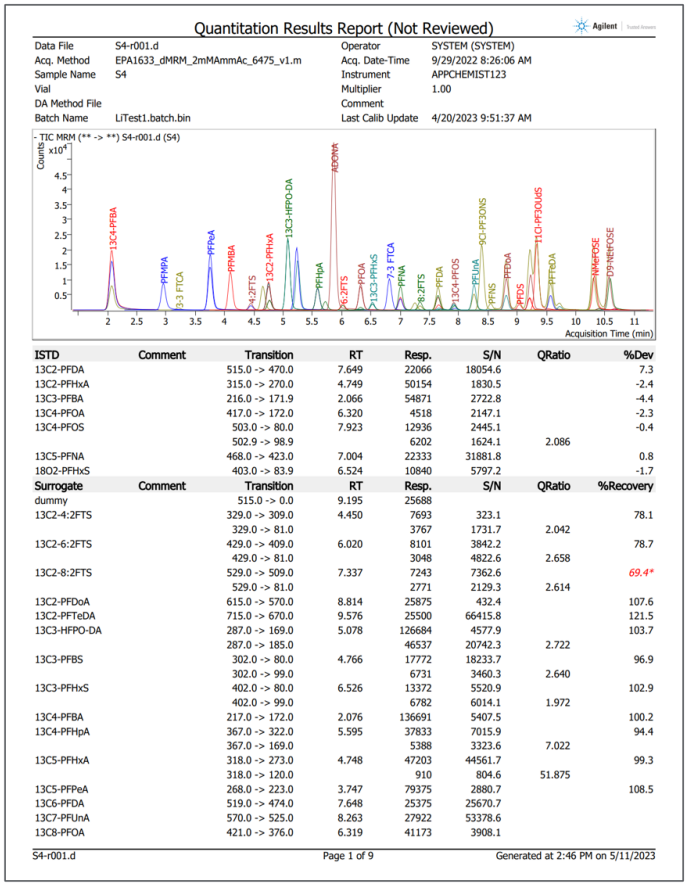


Figure 9. MassHunter Study Manager worklist import screen.


Quantitation Results Report (Not Reviewed)

Agilent

Data File	S4-r001.d	Operator	SYSTEM (SYSTEM)
Acq. Method	EPA1633_dMRM_2mMAmmAc_6475_v1.m	Acq. Date-Time	9/29/2022 8:26:06 AM
Sample Name	S4	Instrument	APPCHEMIST123
Vial		Multiplier	1.00
DA Method File		Comment	
Batch Name	LiTest1.batch.bin	Last Calib Update	4/20/2023 9:51:37 AM

- TIC MRM (** -> **) S4-r001.d (S4)

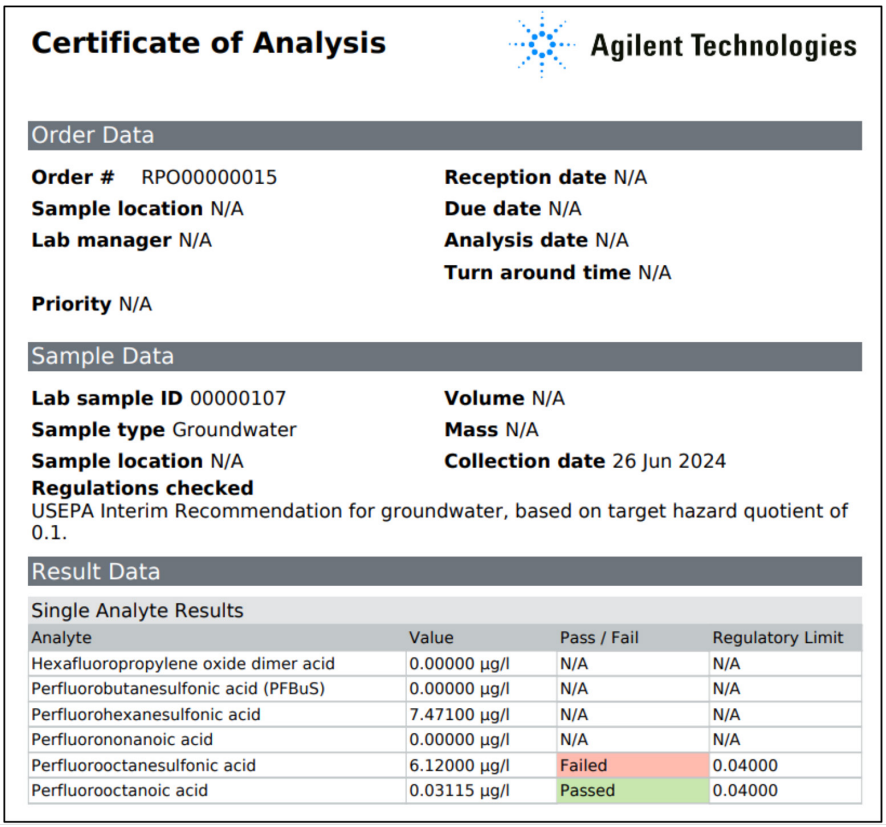
Counts x10^4

Acquisition Time (min)

ISTD	Comment	Transition	RT	Resp.	S/N	QRatio	%Dev
13C2-PFDA		515.0 -> 470.0	7.649	22066	18054.6		7.3
13C2-PFHxA		315.0 -> 270.0	4.749	50154	1830.5		-2.4
13C3-PFBA		216.0 -> 171.9	2.066	54871	2722.8		-4.4
13C4-PFOA		417.0 -> 172.0	6.320	4518	2147.1		-2.3
13C4-PFOS		503.0 -> 80.0	7.923	12936	2445.1		-0.4
		502.9 -> 98.9		6202	1624.1	2.086	
13C5-PFNA		468.0 -> 423.0	7.004	22333	31881.8		0.8
18O2-PFHxS		403.0 -> 83.9	6.524	10840	5797.2		-1.7
Surrogate	**Comment**	**Transition**	**RT**	**Resp.**	**S/N**	**QRatio**	**%Recovery**
dummy		515.0 -> 0.0	9.195	25688			
13C2-4:2FTS		329.0 -> 309.0	4.450	7693	323.1		78.1
		329.0 -> 81.0		3767	1731.7	2.042	
13C2-6:2FTS		429.0 -> 409.0	6.020	8101	3842.2		78.7
		429.0 -> 81.0		3048	4822.6	2.658	
13C2-8:2FTS		529.0 -> 509.0	7.337	7243	7362.6		*69.4**
		529.0 -> 81.0		2771	2129.3	2.614	
13C2-PFDoA		615.0 -> 570.0	8.814	25875	432.4		107.6
13C2-PFTeDA		715.0 -> 670.0	9.576	25500	66415.8		121.5
13C3-HFPO-DA		287.0 -> 169.0	5.078	126684	4577.9		103.7
		287.0 -> 185.0		46537	20742.3	2.722	
13C3-PFBS		302.0 -> 80.0	4.766	17772	18233.7		96.9
		302.0 -> 99.0		6731	3460.3	2.640	
13C3-PFHxS		402.0 -> 80.0	6.526	13372	5520.9		102.9
		402.0 -> 99.0		6782	6014.1	1.972	
13C4-PFBA		217.0 -> 172.0	2.076	136691	5407.5		100.2
13C4-PFHpA		367.0 -> 322.0	5.595	37833	7015.9		94.4
		367.0 -> 169.0		5388	3323.6	7.022	
13C5-PFHxA		318.0 -> 273.0	4.748	47203	44561.7		99.3
		318.0 -> 120.0		910	804.6	51.875	
13C5-PFPeA		268.0 -> 223.0	3.747	79375	2880.7		108.5
13C6-PFDA		519.0 -> 474.0	7.648	25375	25670.7		
13C7-PFUnA		570.0 -> 525.0	8.263	27922	53378.6		
13C8-PFOA		421.0 -> 376.0	6.319	41173	3908.1		

S4-r001.d Page 1 of 9 Generated at 2:46 PM on 5/11/2023

Figure 10. Part of the Quantitation Results Report generated by MassHunter.



Certificate of Analysis

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Order Data

Order # RPO00000015
Sample location N/A
Lab manager N/A
Priority N/A
Reception date N/A
Due date N/A
Analysis date N/A
Turn around time N/A

Sample Data

Lab sample ID 00000107
Sample type Groundwater
Sample location N/A
Volume N/A
Mass N/A
Collection date 26 Jun 2024
Regulations checked
USEPA Interim Recommendation for groundwater, based on target hazard quotient of 0.1.

Result Data

Single Analyte Results

Analyte	Value	Pass / Fail	Regulatory Limit
Hexafluoropropylene oxide dimer acid	0.00000 µg/l	N/A	N/A
Perfluorobutanesulfonic acid (PFBuS)	0.00000 µg/l	N/A	N/A
Perfluorohexanesulfonic acid	7.47100 µg/l	N/A	N/A
Perfluorononanoic acid	0.00000 µg/l	N/A	N/A
Perfluorooctanesulfonic acid	6.12000 µg/l	Failed	0.04000
Perfluorooctanoic acid	0.03115 µg/l	Passed	0.04000

Figure 11. Part of the Certificate of Analysis generated by SLIMS with Pass/Fail evaluated.

Summary

Agilent SLIMS transforms PFAS testing by centralizing critical lab functions into a single, intuitive platform. By integrating sample tracking, inventory management, digital protocols and reporting, SLIMS enhances operational efficiency, ensures data integrity, and supports regulatory compliance. This powerful tool simplifies complex workflows, enabling laboratories to achieve faster, more accurate results, resulting in a more efficient PFAS analysis. With its ability to easily integrate with existing lab systems and provide real-time updates, SLIMS is essential for labs aiming to meet stringent regulatory standards and maintain high productivity.

References

1. United States Environmental Protection Agency Method 1633. https://www.epa.gov/system/files/documents/2024-01/method-1633-final-for-web-posting.pdf
2. Hunt, K., Hindle, R. (Vogon Laboratory Services Ltd., Cochrane, AB, Canada), Anumol, T., Giardina, M., Juck, M., and Parry, E. (Agilent Technologies, Inc.). Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Aqueous Samples Per EPA Method 1633. Agilent Technologies application note, publication number 5994-5226EN, 2024.
3. Giardina, M. and Juck, M. (Agilent Technologies). Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Solid Samples. Agilent Technologies application note, publication number 5994-5667EN, 2023.

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