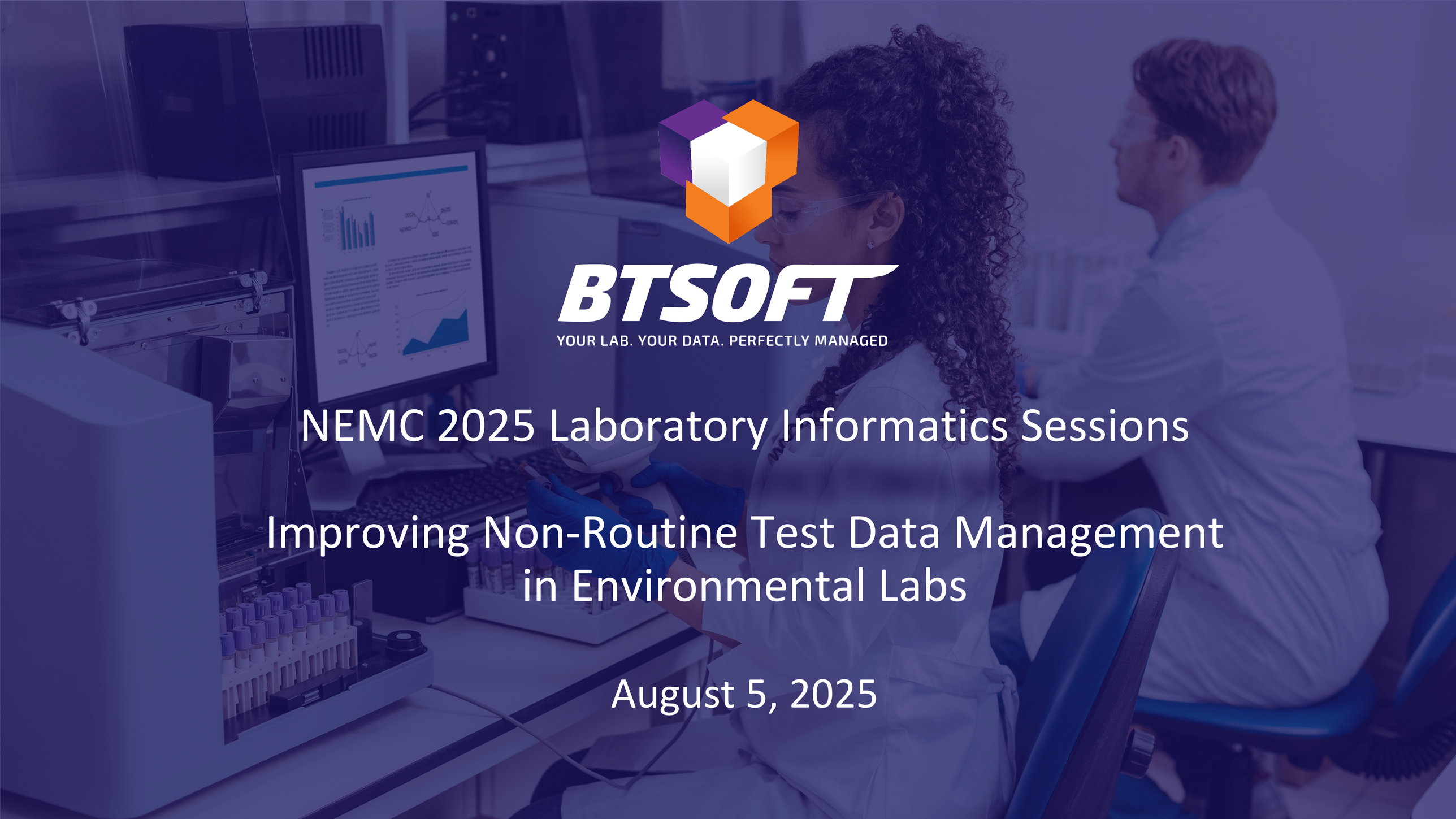

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NEMC 2025 Laboratory Informatics Sessions

Improving Non-Routine Test Data Management in Environmental Labs

August 5, 2025

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Introduction

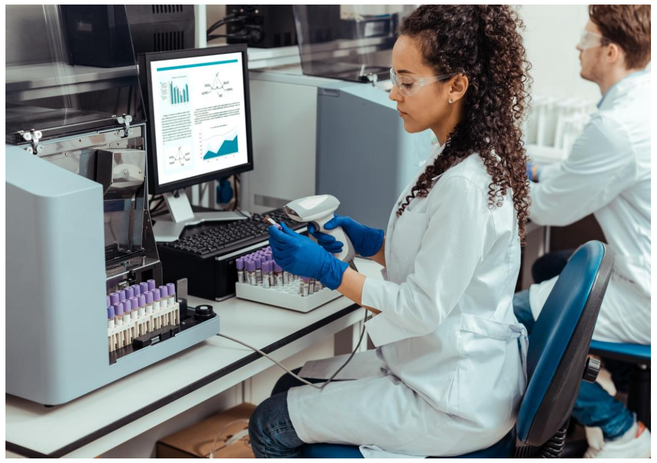
Environmental laboratories are equipped to perform a wide range of standardized analyses across various matrices. While routine tests are well-supported by existing Laboratory Information Management Systems (LIMS), specialized analyses—such as flashpoint, corrosivity, chlorophyll, and marine organism testing—often lack the same level of workflow integration.

This presentation explores the data management challenges associated with non-routine testing and introduces solutions that enhance traceability, efficiency, and regulatory compliance.

Common Laboratory Testing

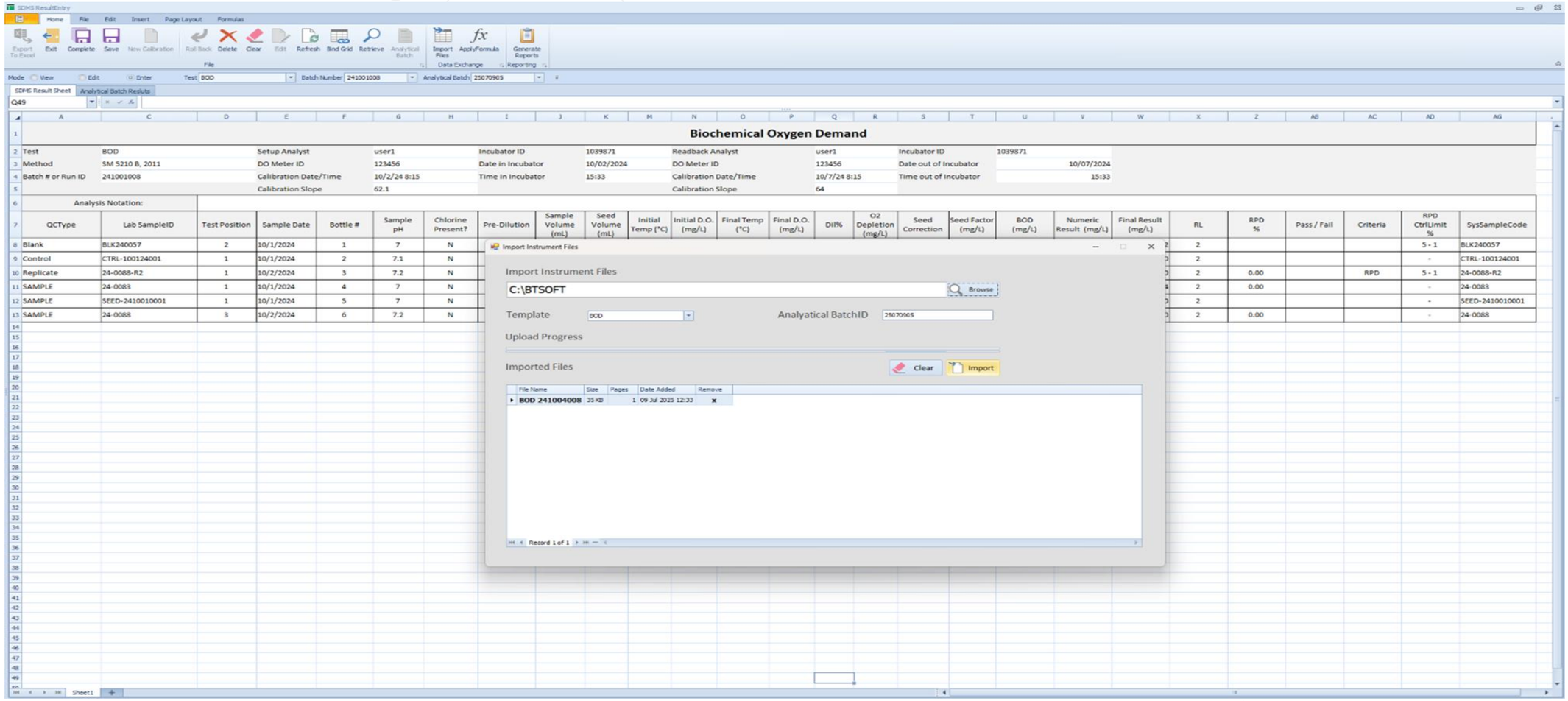
- Environmental laboratories frequently perform standard tests across various matrices:
- - Wet chemistry for inorganic substances
- - Metals content analysis
- - Volatile and semi-volatile organic analysis

- However, challenges can arise with non-routine test data collection and storage.



Common Laboratory Testing (BOD5)

- While SDMS addresses non-routine testing gaps, it is equally effective in supporting routine, high-volume analyses—offering efficiency and consistency across all workflows.



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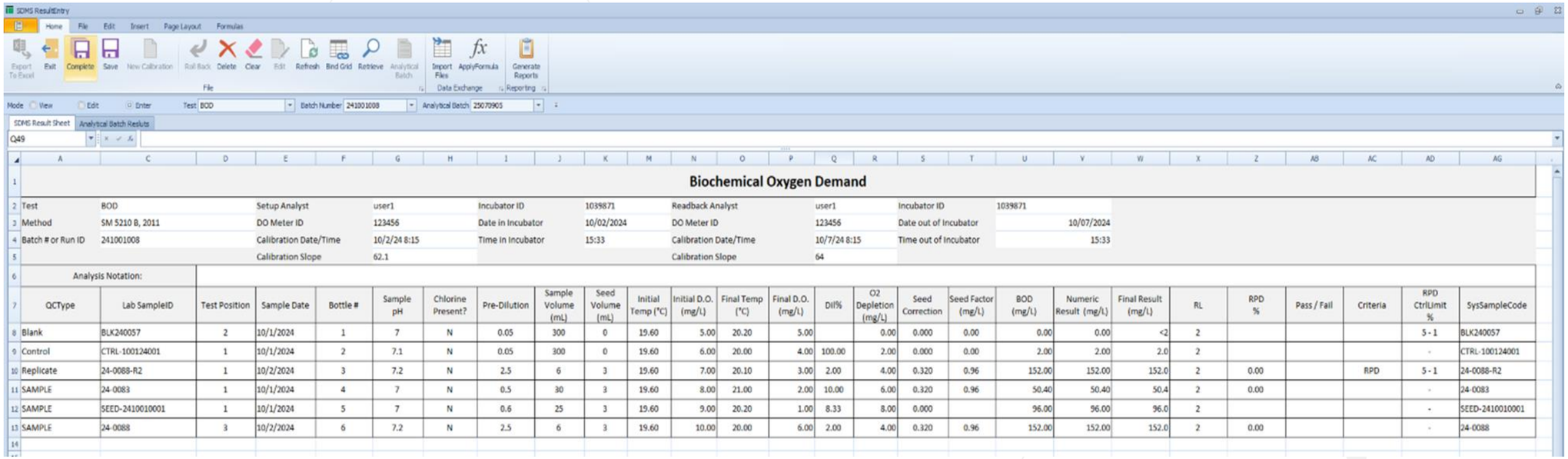
Common Laboratory Testing (BOD5)

- SDMS does not have to replace existing systems but complements any LIMS by extending its capability to manage flexible, template-driven, and traceable data entry.



Biochemical Oxygen Demand

Test	BOD	Setup Analyst	user1	Incubator ID	1039871	Readback Analyst	user1
Method	SM 5210 B, 2011	DO Meter ID	123456	Date in Incubator	10/02/2024	DO Meter ID	123456
Batch # or Run ID	241001008	Calibration Date/Time	10/2/24 8:15	Time in Incubator	15:33	Calibration Date/Time	10/7/24 8:15
		Calibration Slope	62.1			Calibration Slope	64

Analysis Notation:																										
QCType	Lab SampleID	Test Position	Sample Date	Bottle #	Sample pH	Chlorine Present?	Pre-Dilution	Sample Volume (mL)	Seed Volume (mL)	Initial Temp (°C)	Initial D.O. (mg/L)	Final Temp (°C)	Final D.O. (mg/L)	Dil%	O2 Depletion (mg/L)	Seed Correction	Seed Factor (mg/L)	BOD (mg/L)	Numeric Result (mg/L)	Final Result (mg/L)	RL	RPD %	Pass / Fail	Criteria	RPD CtrlLimit %	SysSampleCode
Blank	BLK240057	2	10/1/2024	1	7	N	0.05	300	0	19.60	5.00	20.20	5.00		0.00	0.000	0.00	0.00	0.00	<2	2				5 - 1	BLK240057
Control	CTRL-100124001	1	10/1/2024	2	7.1	N	0.05	300	0	19.60	6.00	20.00	4.00	100.00	2.00	0.000	0.00	2.00	2.00	2.0	2				-	CTRL-100124001
Replicate	24-0088-R2	1	10/2/2024	3	7.2	N	2.5	6	3	19.60	7.00	20.10	3.00	2.00	4.00	0.320	0.96	152.00	152.00	152.0	2	0.00		RPD	5 - 1	24-0088-R2
SAMPLE	24-0083	1	10/1/2024	4	7	N	0.5	30	3	19.60	8.00	21.00	2.00	10.00	6.00	0.320	0.96	50.40	50.40	50.4	2	0.00			-	24-0083
SAMPLE	SEED-2410010001	1	10/1/2024	5	7	N	0.6	25	3	19.60	9.00	20.20	1.00	8.33	8.00	0.000		96.00	96.00	96.0	2				-	SEED-2410010001
SAMPLE	24-0088	3	10/2/2024	6	7.2	N	2.5	6	3	19.60	10.00	20.00	6.00	2.00	4.00	0.320	0.96	152.00	152.00	152.0	2	0.00			-	24-0088

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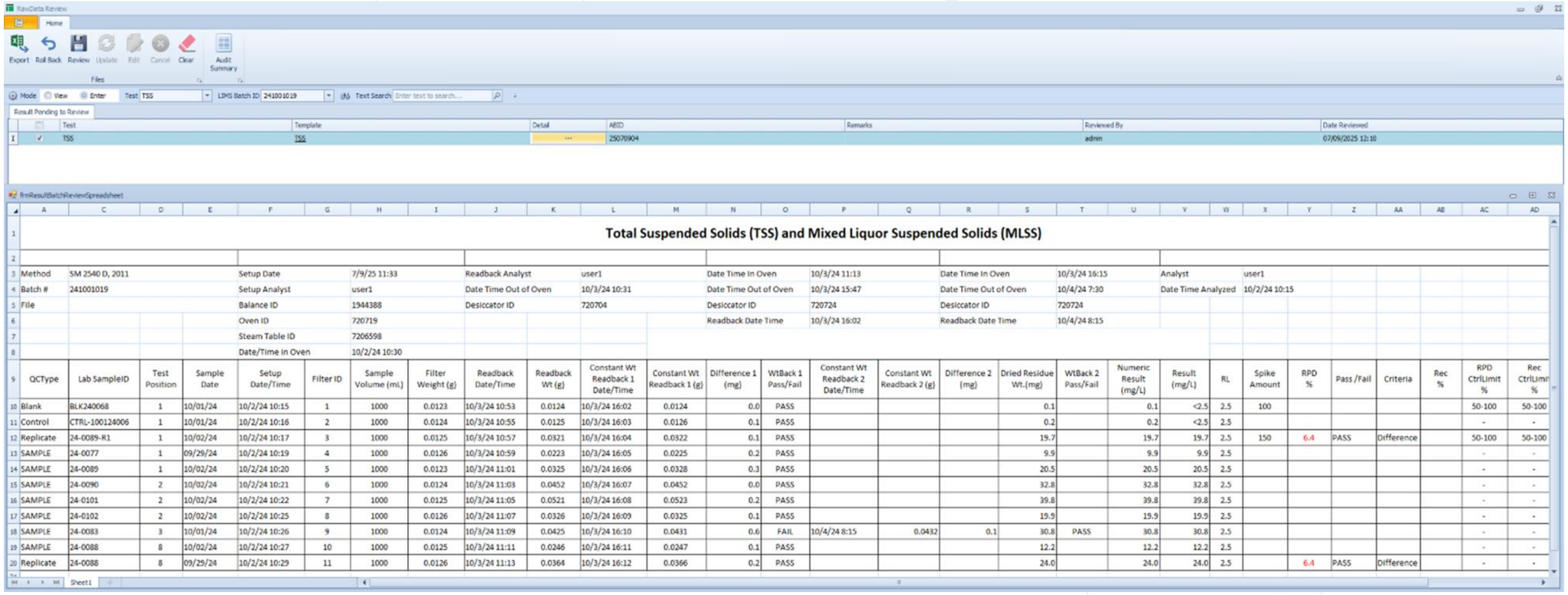
Common Laboratory Testing (TSS/MLSS)

- SDMS directly contributes to laboratory digitalization by eliminating paper-based processes, enhancing data integrity, and simplifying audits.



RawData Review

Home

Export | Roll Back | Review | Update | Edit | Cancel | Clear | Audit Summary

Files

Mode: View / Enter | Test: TSS | LIMS Batch ID: 241001019 | Text Search: Enter text to search...

Result Pending to Review

	Test	Template	Detail	AEID	Remarks	Reviewed By	Date Reviewed
I	TSS	TSS	...	25070904		admin	07/09/2025 12:10

frmResultBatchReviewSpreadsheet

Total Suspended Solids (TSS) and Mixed Liquor Suspended Solids (MLSS)

Method	SM 2540 D, 2011	Setup Date	7/9/25 11:33	Readback Analyst	user1	Date Time In Oven	10/3/24 11:13	Date Time In Oven	10/3/24 16:15	Analyst	user1
Batch #	241001019	Setup Analyst	user1	Date Time Out of Oven	10/3/24 10:31	Date Time Out of Oven	10/3/24 15:47	Date Time Out of Oven	10/4/24 7:30	Date Time Analyzed	10/2/24 10:15
File		Balance ID	1944388	Desiccator ID	720704	Desiccator ID	720724	Desiccator ID	720724		
		Oven ID	720719			Readback Date Time	10/3/24 16:02	Readback Date Time	10/4/24 8:15		
		Steam Table ID	7206598								
		Date/Time In Oven	10/2/24 10:30								

QCType	Lab SampleID	Test Position	Sample Date	Setup Date/Time	Filter ID	Sample Volume (mL)	Filter Weight (g)	Readback Date/Time	Readback Wt (g)	Constant Wt Readback 1 Date/Time	Constant Wt Readback 1 (g)	Difference 1 (mg)	WtBack 1 Pass/Fail	Constant Wt Readback 2 Date/Time	Constant Wt Readback 2 (g)	Difference 2 (mg)	Dried Residue Wt.(mg)	WtBack 2 Pass/Fail	Numeric Result (mg/L)	Result (mg/L)	RL	Spike Amount	RPD %	Pass /Fail	Criteria	Rec %	RPD CtrlLimit %	Rec CtrlLimit %
Blank	BLK240068	1	10/01/24	10/2/24 10:15	1	1000	0.0123	10/3/24 10:53	0.0124	10/3/24 16:02	0.0124	0.0	PASS				0.1		0.1	<2.5	2.5	100					50-100	50-100
Control	CTRL-100124006	1	10/01/24	10/2/24 10:16	2	1000	0.0124	10/3/24 10:55	0.0125	10/3/24 16:03	0.0126	0.1	PASS				0.2		0.2	<2.5	2.5						-	-
Replicate	24-0089-R1	1	10/02/24	10/2/24 10:17	3	1000	0.0125	10/3/24 10:57	0.0321	10/3/24 16:04	0.0322	0.1	PASS				19.7		19.7	19.7	2.5	150	6.4	PASS	Difference		50-100	50-100
SAMPLE	24-0077	1	09/29/24	10/2/24 10:19	4	1000	0.0126	10/3/24 10:59	0.0223	10/3/24 16:05	0.0225	0.2	PASS				9.9		9.9	9.9	2.5						-	-
SAMPLE	24-0089	1	10/02/24	10/2/24 10:20	5	1000	0.0123	10/3/24 11:01	0.0325	10/3/24 16:06	0.0328	0.3	PASS				20.5		20.5	20.5	2.5						-	-
SAMPLE	24-0090	2	10/02/24	10/2/24 10:21	6	1000	0.0124	10/3/24 11:03	0.0452	10/3/24 16:07	0.0452	0.0	PASS				32.8		32.8	32.8	2.5						-	-
SAMPLE	24-0101	2	10/02/24	10/2/24 10:22	7	1000	0.0125	10/3/24 11:05	0.0521	10/3/24 16:08	0.0523	0.2	PASS				39.8		39.8	39.8	2.5						-	-
SAMPLE	24-0102	2	10/02/24	10/2/24 10:25	8	1000	0.0126	10/3/24 11:07	0.0326	10/3/24 16:09	0.0325	0.1	PASS				19.9		19.9	19.9	2.5						-	-
SAMPLE	24-0083	3	10/01/24	10/2/24 10:26	9	1000	0.0124	10/3/24 11:09	0.0425	10/3/24 16:10	0.0431	0.6	FAIL	10/4/24 8:15	0.0432	0.1	30.8	PASS	30.8	30.8	2.5						-	-
SAMPLE	24-0088	8	10/02/24	10/2/24 10:27	10	1000	0.0125	10/3/24 11:11	0.0246	10/3/24 16:11	0.0247	0.1	PASS				12.2		12.2	12.2	2.5						-	-
Replicate	24-0088	8	09/29/24	10/2/24 10:29	11	1000	0.0126	10/3/24 11:13	0.0364	10/3/24 16:12	0.0366	0.2	PASS				24.0		24.0	24.0	2.5		6.4	PASS	Difference		-	-

Sheet1

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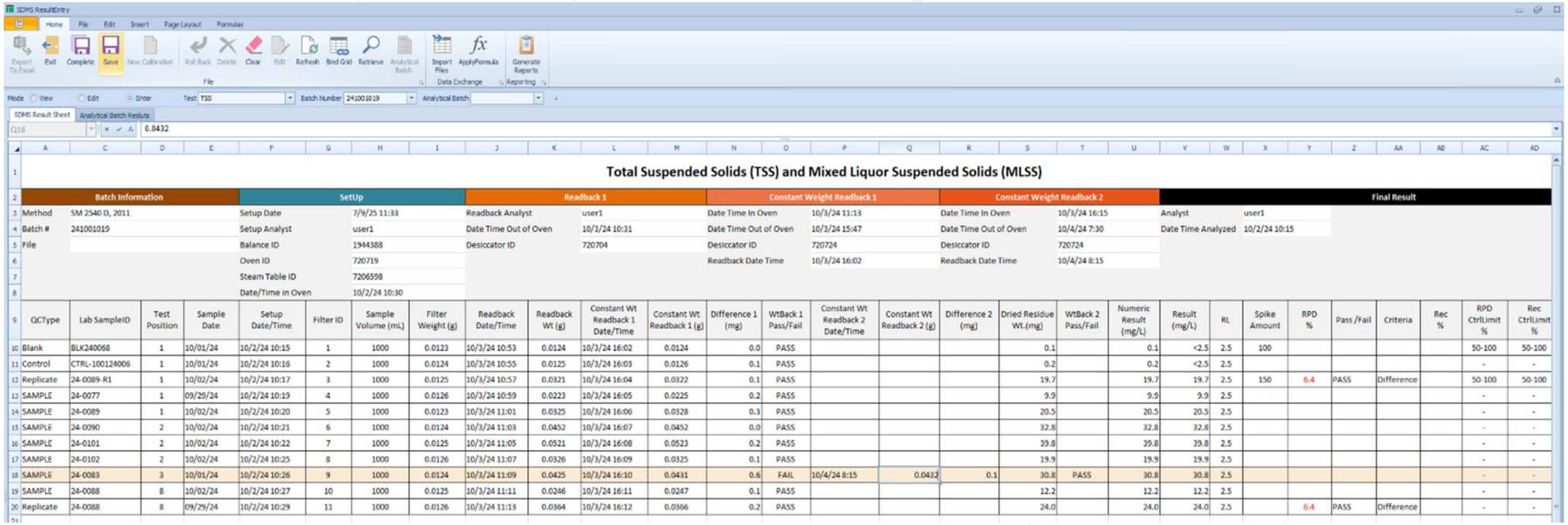
Common Laboratory Testing (TSS/MLSS)

- Workflows such as DF selection, duplicate tracking, and review steps can be configured per template—no code required.



Total Suspended Solids (TSS) and Mixed Liquor Suspended Solids (MLSS)

Batch Information		SetUp		Readback 1		Constant Weight Readback 1		Constant Weight Readback 2		Final Result	
Method	SM 2540 D, 2011	Setup Date	7/9/25 11:33	Readback Analyst	user1	Date Time In Oven	10/3/24 11:13	Date Time In Oven	10/3/24 16:15	Analyst	user1
Batch #	241001019	Setup Analyst	user1	Date Time Out of Oven	10/3/24 10:31	Date Time Out of Oven	10/3/24 15:47	Date Time Out of Oven	10/4/24 7:30	Date Time Analyzed	10/2/24 10:15
File		Balance ID	1944388	Desiccator ID	720704	Desiccator ID	720724	Desiccator ID	720724		
		Oven ID	720719			Readback Date Time	10/3/24 16:02	Readback Date Time	10/4/24 8:15		
		Steam Table ID	7206598								
		Date/Time in Oven	10/2/24 10:30								

QCType	Lab SampleID	Test Position	Sample Date	Setup Date/Time	Filter ID	Sample Volume (mL)	Filter Weight (g)	Readback Date/Time	Readback Wt (g)	Constant Wt Readback 1 Date/Time	Constant Wt Readback 1 (g)	Difference 1 (mg)	WtBack 1 Pass/Fail	Constant Wt Readback 2 Date/Time	Constant Wt Readback 2 (g)	Difference 2 (mg)	Dried Residue Wt.(mg)	WtBack 2 Pass/Fail	Numeric Result (mg/L)	Result (mg/L)	RL	Spike Amount	RPD %	Pass /Fail	Criteria	Rec %	RPD CtrlLimit %	Rec CtrlLimit %
Blank	BLK240068	1	10/01/24	10/2/24 10:15	1	1000	0.0123	10/3/24 10:53	0.0124	10/3/24 16:02	0.0124	0.0	PASS				0.1		0.1	<2.5	2.5	100					50-100	50-100
Control	CTRL-100124006	1	10/01/24	10/2/24 10:16	2	1000	0.0124	10/3/24 10:55	0.0125	10/3/24 16:03	0.0126	0.1	PASS				0.2		0.2	<2.5	2.5						-	-
Replicate	24-0089-R1	1	10/02/24	10/2/24 10:17	3	1000	0.0125	10/3/24 10:57	0.0321	10/3/24 16:04	0.0322	0.1	PASS				19.7		19.7	19.7	2.5	150	6.4	PASS	Difference		50-100	50-100
SAMPLE	24-0077	1	09/29/24	10/2/24 10:19	4	1000	0.0126	10/3/24 10:59	0.0223	10/3/24 16:05	0.0225	0.2	PASS				9.9		9.9	9.9	2.5						-	-
SAMPLE	24-0089	1	10/02/24	10/2/24 10:20	5	1000	0.0123	10/3/24 11:01	0.0325	10/3/24 16:06	0.0328	0.3	PASS				20.5		20.5	20.5	2.5						-	-
SAMPLE	24-0090	2	10/02/24	10/2/24 10:21	6	1000	0.0124	10/3/24 11:03	0.0452	10/3/24 16:07	0.0452	0.0	PASS				32.8		32.8	32.8	2.5						-	-
SAMPLE	24-0101	2	10/02/24	10/2/24 10:22	7	1000	0.0125	10/3/24 11:05	0.0521	10/3/24 16:08	0.0523	0.2	PASS				39.8		39.8	39.8	2.5						-	-
SAMPLE	24-0102	2	10/02/24	10/2/24 10:25	8	1000	0.0126	10/3/24 11:07	0.0326	10/3/24 16:09	0.0325	0.1	PASS				19.9		19.9	19.9	2.5						-	-
SAMPLE	24-0083	3	10/01/24	10/2/24 10:26	9	1000	0.0124	10/3/24 11:09	0.0425	10/3/24 16:10	0.0431	0.6	FAIL	10/4/24 8:15	0.0432	0.1	30.8	PASS	30.8	30.8	2.5						-	-
SAMPLE	24-0088	8	10/02/24	10/2/24 10:27	10	1000	0.0125	10/3/24 11:11	0.0246	10/3/24 16:11	0.0247	0.1	PASS				12.2		12.2	12.2	2.5						-	-
Replicate	24-0088	8	09/29/24	10/2/24 10:29	11	1000	0.0126	10/3/24 11:13	0.0364	10/3/24 16:12	0.0366	0.2	PASS				24.0		24.0	24.0	2.5		6.4	PASS	Difference		-	-

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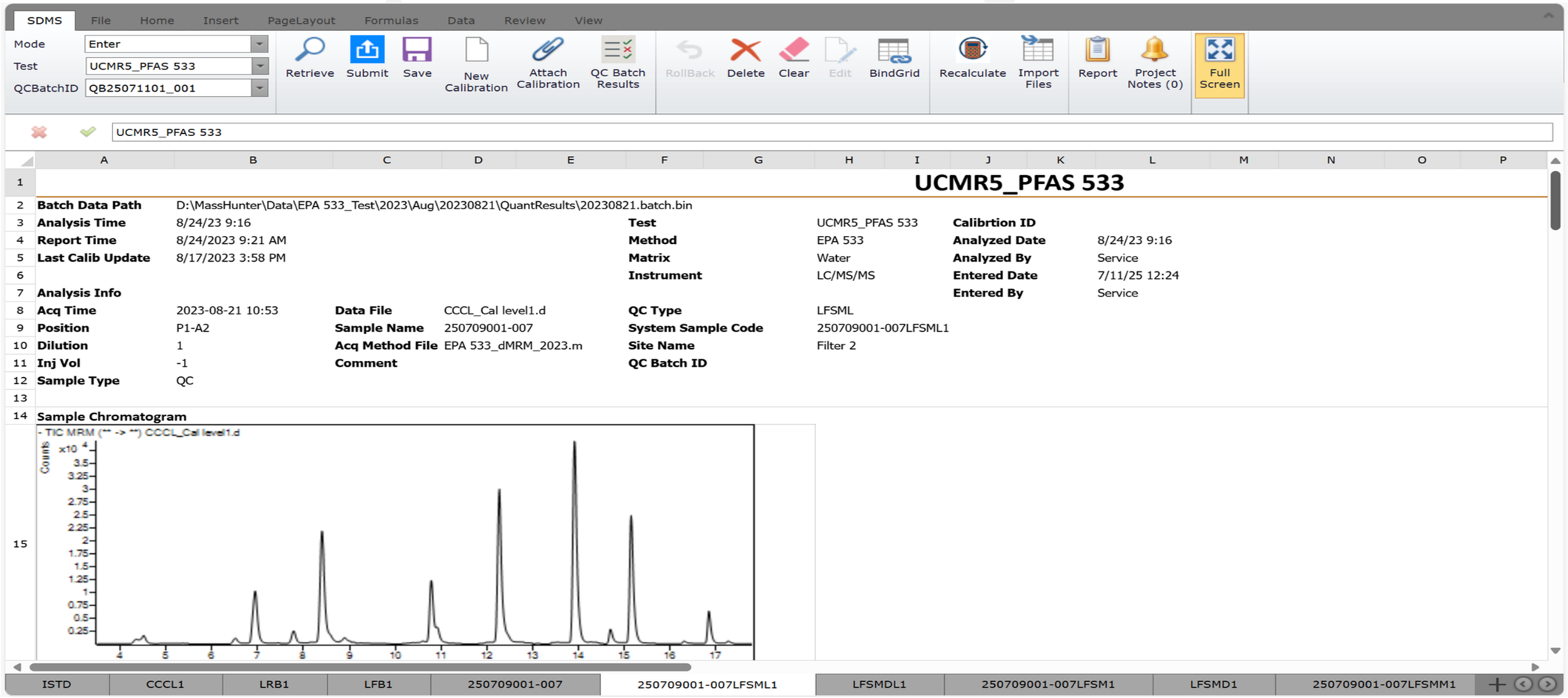
Common Laboratory Testing (UCMR5 PFAS 533)

- Users can create and deploy customized result entry templates tailored to their workflows and regulations—without any programming effort.



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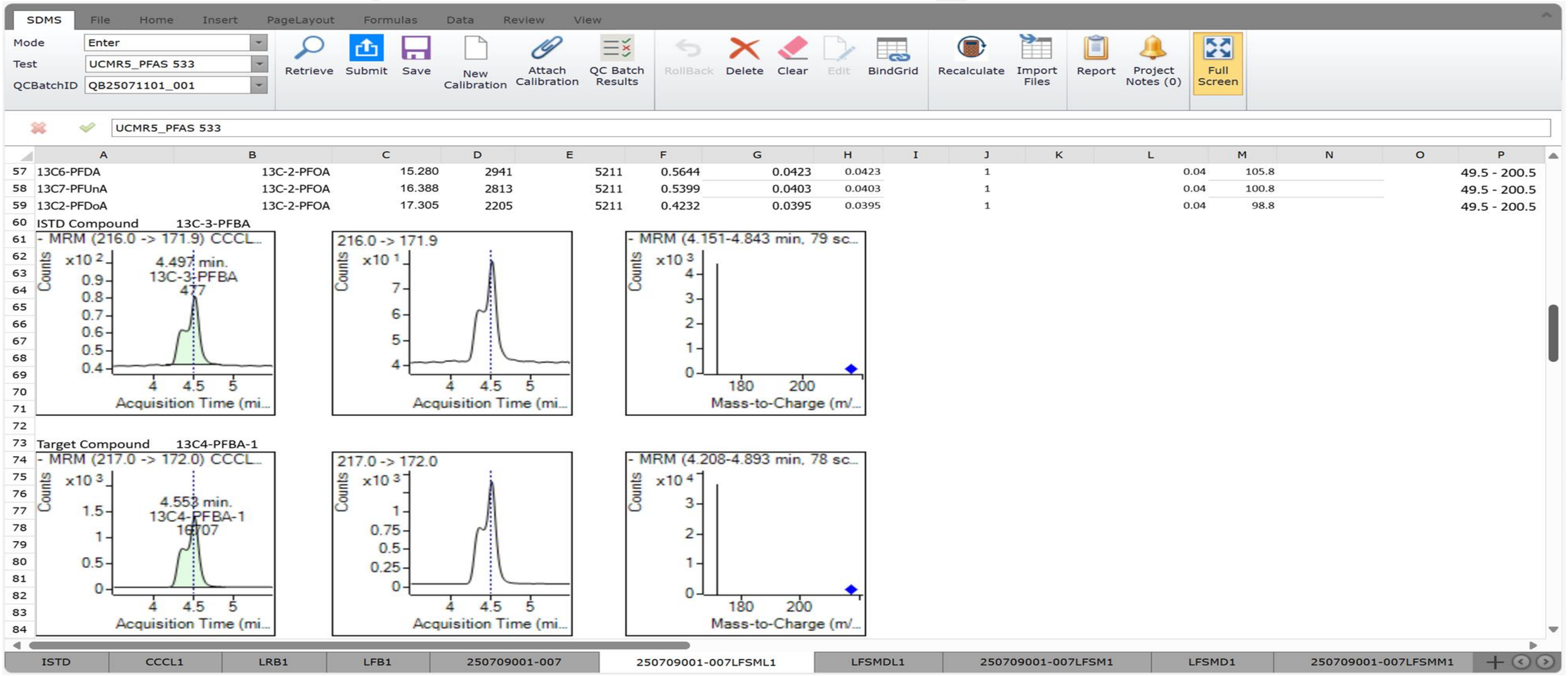
Common Laboratory Testing (UCMR5 PFAS 533)

- Automatic flagging, built-in formulas, and configurable validation rules make SDMS a quality-centric system suitable for regulated environments.



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Challenges with Non-Routine Tests

Examples of non-routine tests:

- - Phytoplankton
- - Particle Size Distribution
- - Chlorophyll
- - Ocean Currents

Issues:

- - Lack of specific workflows in LIMS
- - Inefficient and non-traceable data methods
- - Use of customized spreadsheets leads to errors and non-compliance

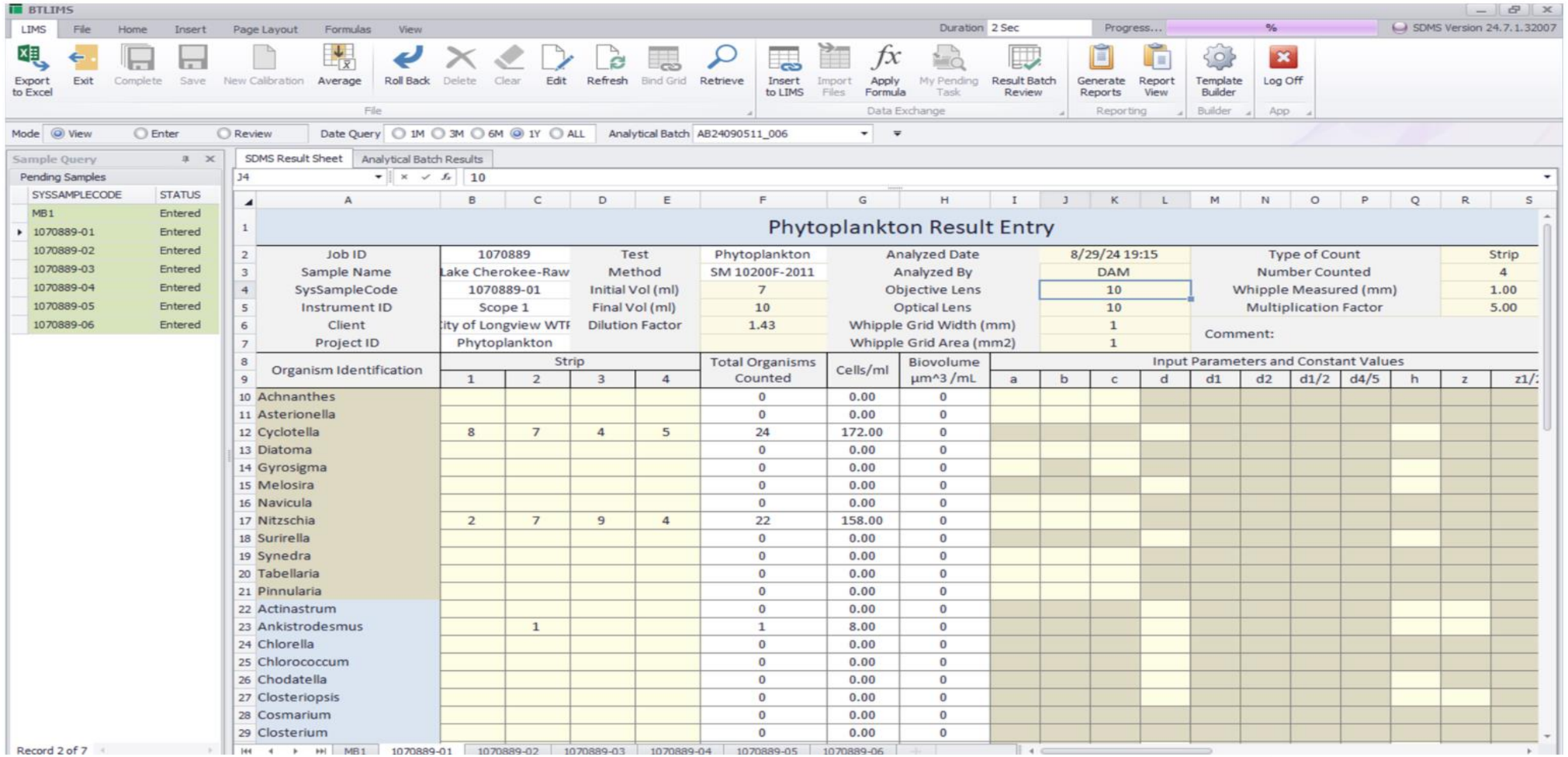
Solution – Sample Data Management System (SDMS)

Key benefits of SDMS:

- - LIMS-agnostic system for managing all lab testing data
- - Automates electronic data capture
- - Replaces spreadsheets with reliable processes
- - Supports informatics-style solutions for non-routine analyses

Challenges with Non-Routine Tests (Ex: Marine Organisms)

- Every action—entry, edit, approval—is logged and traceable, ensuring data accountability and regulatory readiness.



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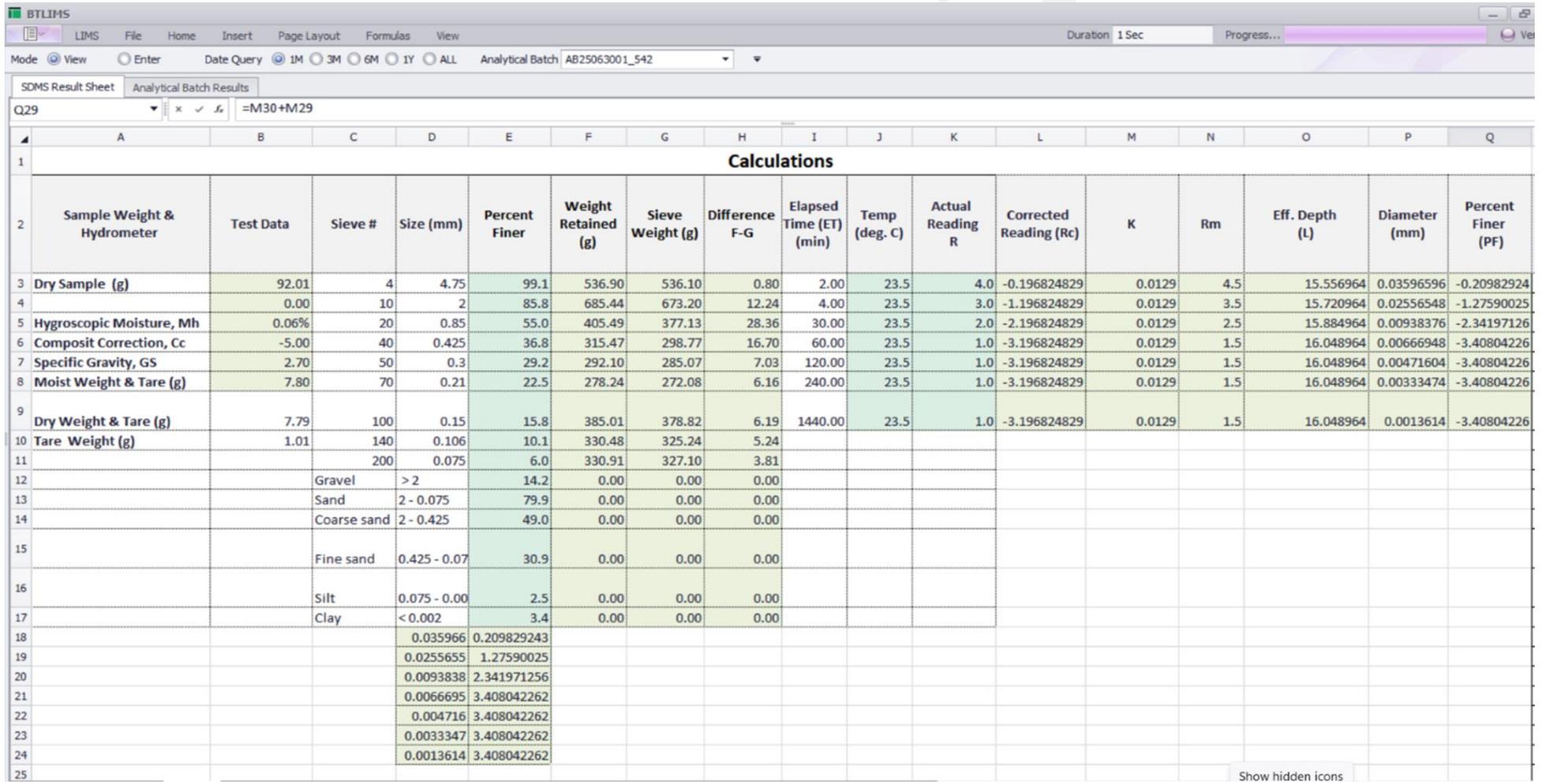
Challenges with Non-Routine Tests (Ex: Particle Size Distribution)

- SDMS connects instruments, exports to LIMS, and supports EDD/reporting with minimal integration effort.



Calculations

Sample Weight & Hydrometer	Test Data	Sieve #	Size (mm)	Percent Finer	Weight Retained (g)	Sieve Weight (g)	Difference F-G	Elapsed Time (ET) (min)	Temp (deg. C)	Actual Reading R	Corrected Reading (Rc)	K	Rm	Eff. Depth (L)	Diameter (mm)	Percent Finer (PF)
Dry Sample (g)	92.01	4	4.75	99.1	536.90	536.10	0.80	2.00	23.5	4.0	-0.196824829	0.0129	4.5	15.556964	0.03596596	-0.20982924
	0.00	10	2	85.8	685.44	673.20	12.24	4.00	23.5	3.0	-1.196824829	0.0129	3.5	15.720964	0.02556548	-1.27590025
Hygroscopic Moisture, Mh	0.06%	20	0.85	55.0	405.49	377.13	28.36	30.00	23.5	2.0	-2.196824829	0.0129	2.5	15.884964	0.00938376	-2.34197126
Composit Correction, Cc	-5.00	40	0.425	36.8	315.47	298.77	16.70	60.00	23.5	1.0	-3.196824829	0.0129	1.5	16.048964	0.00666948	-3.40804226
Specific Gravity, GS	2.70	50	0.3	29.2	292.10	285.07	7.03	120.00	23.5	1.0	-3.196824829	0.0129	1.5	16.048964	0.00471604	-3.40804226
Moist Weight & Tare (g)	7.80	70	0.21	22.5	278.24	272.08	6.16	240.00	23.5	1.0	-3.196824829	0.0129	1.5	16.048964	0.00333474	-3.40804226
Dry Weight & Tare (g)	7.79	100	0.15	15.8	385.01	378.82	6.19	1440.00	23.5	1.0	-3.196824829	0.0129	1.5	16.048964	0.0013614	-3.40804226
Tare Weight (g)	1.01	140	0.106	10.1	330.48	325.24	5.24									
		200	0.075	6.0	330.91	327.10	3.81									
		Gravel	> 2	14.2	0.00	0.00	0.00									
		Sand	2 - 0.075	79.9	0.00	0.00	0.00									
		Coarse sand	2 - 0.425	49.0	0.00	0.00	0.00									
		Fine sand	0.425 - 0.07	30.9	0.00	0.00	0.00									
		Silt	0.075 - 0.00	2.5	0.00	0.00	0.00									
		Clay	< 0.002	3.4	0.00	0.00	0.00									
			0.035966	0.209829243												
			0.0255655	1.27590025												
			0.0093838	2.341971256												
			0.0066695	3.408042262												
			0.004716	3.408042262												
			0.0033347	3.408042262												
			0.0013614	3.408042262												

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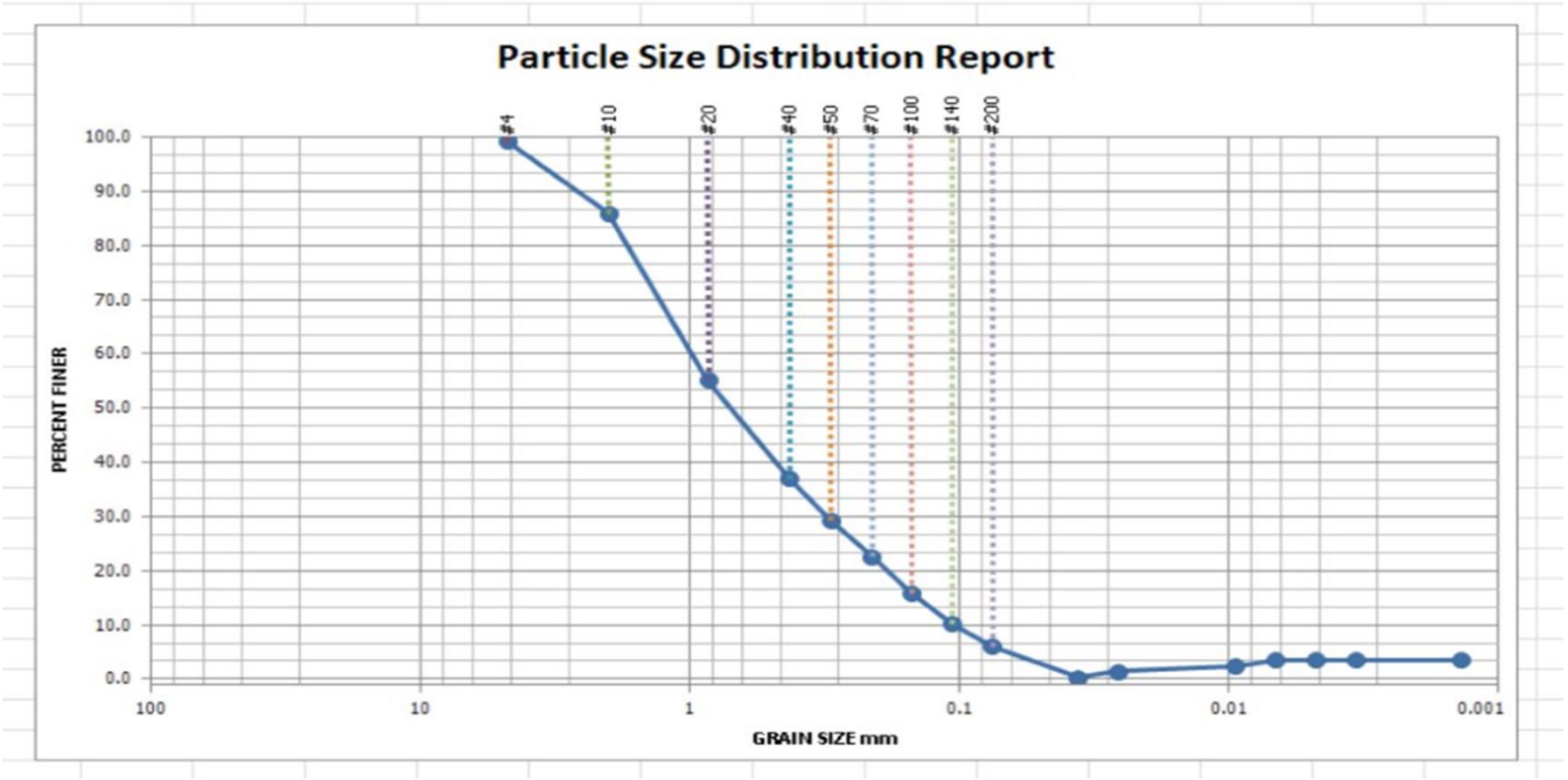
Challenges with Non-Routine Tests (Ex: Particle Size Distribution)

- Though designed for environmental labs, SDMS applies to many laboratory sectors, including Consumer Products, Food, Agriculture, and Industrial testing.



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Conclusion and Potential Next Steps

Summary:

- Non-routine and specialized testing are critical yet often overlooked aspects of laboratory data management.
- Traditional methods like spreadsheets create inefficiencies, risk errors, and hinder compliance.
- Implementing an SDMS provides a scalable, reliable, and LIMS-independent solution for managing all test data.

Next Steps:

1. Assess your lab’s current data collection processes.
2. Identify gaps in non-routine test data workflows.
3. Explore SDMS solutions that integrate with your existing systems to improve compliance and traceability.