Utilizing Automated Data Review to Evaluate Large Data Sets at Los Alamos National Laboratory

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** -- Presenter*

Driving Cleanup ▪ Honoring the Past ▪ Strengthening Communities

Outline

- Introduction
- Sample / Data Flow
- Automated Data Review
- Level 3 Validation
- Summary

Introduction

- **Newport News Nuclear BWXT-Los Alamos, LLC (N3B)**
  - Owned by Newport News Nuclear, a division of Huntington Ingalls Industries and BWX Technologies
  - Implements the Los Alamos Legacy Cleanup Contract (LLCC) for the U.S. Department of Energy, Environmental Management, Los Alamos Field Office (DOE EM-LA)
  - Responsible for clean-up of Manhattan Project and Cold War Legacy Waste and contamination at Los Alamos National Laboratory (LANL)

Introduction

- ~10,000 samples collected annually
  - Routine ground water monitoring
  - Regulatory surface water monitoring
  - Annual Site Environmental Report surface water and sediment sampling
  - Soil remediation projects
  - Soil vapor monitoring of material disposal areas
  - Waste characterization

- Utilize Locus Environmental Information Management (EIM) software for data management
- Environmental data publicly available on IntellusNM.com

N3B Data Management

- N3B's Sample and Data Management Team's data management principles:

1. Defensibility
   A. Chain of custody

2. High Quality
   A. DOECAP assessed analytical laboratories
   B. Procedure driven
   C. Expert chemists

3. Efficiency
   A. Automation where possible
      I. Mobile sample collection logs
      II. Electronic lab log-in sheets
      III. Automated data review

N3B Data Management

- Samples collected
- Samples analyzed at external laboratory
- Data loaded into EIM holding table
- Examination and verification occurs in holding table
- Data pushed to final tables and available for querying
- Manual validation occurs offline, with updated qualifications uploaded back into the system

Introduction

- Typical Analytical Suite
  - Volatile Organic Compounds (~80 parameters)
  - Semi-Volatile Compounds (~80 Parameters)
  - High Explosives (~20 Parameters)
  - Perchlorate
  - PCB Aroclors (8 parameters)
  - Metals (~25 Parameters)
  - General Chemistry (~15 Parameters)
  - Radiochemistry (~20 Parameters)

(Approximately 250 Parameters/Sample)

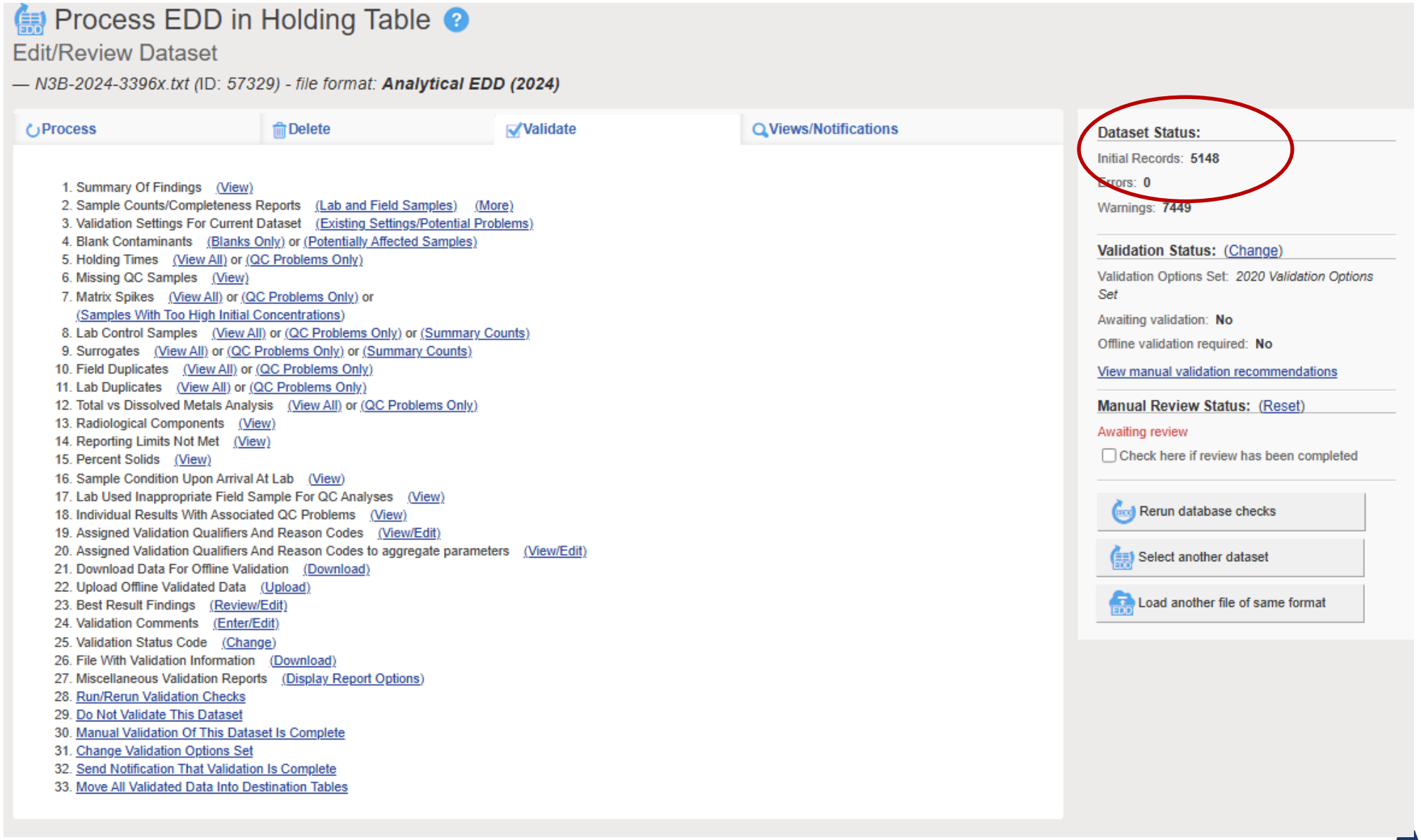
Approximately 10 Samples per data set

During the 2024 summer campaign, it was not uncommon to have 10 data sets of this size delivered by the lab on any given day

2500 Analytical records just from field sample target analytes

Including all QC records, it is not uncommon for the chemist to have to review over 4000 records for one data set

EIM Automated Data Review



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EIM Automated Data Review – Quality Control

Process EDD in Holding Table

Edit/Review Dataset

— *N3B-2025-2500_test.txt* (ID: *60900*) - *file format:* ***Analytical EDD (2025)***

Process | Delete | Validate

1. Summary Of Findings (View)
2. Sample Counts/Completeness Reports (Lab and Field Samples) (More)
3. Validation Settings For Current Dataset (Existing Settings/Potential Problems)
4. Blank Contaminants (Blanks Only) or (Potentially Affected Samples)
5. Holding Times (View All) or (QC Problems Only)
6. Missing QC Samples (View)
7. Matrix Spikes (View All) or (QC Problems Only) or (Samples With Too High Initial Concentrations)
8. Lab Control Samples (View All) or (QC Problems Only) or (Summary Counts)
9. Surrogates (View All) or (QC Problems Only) or (Summary Counts)
10. Field Duplicates (View All) or (QC Problems Only)
11. Lab Duplicates (View All) or (QC Problems Only)
12. Total vs Dissolved Metals Analysis (View All) or (QC Problems Only)
13. Radiological Components (View)
14. Reporting Limits Not Met (View)
15. Percent Solids (View)
16. Sample Condition Upon Arrival At Lab (View)
17. Lab Used Inappropriate Field Sample For QC Analyses (View)
18. Individual Results With Associated QC Problems (View)
19. Assigned Validation Qualifiers And Reason Codes (View/Edit)
20. Assigned Validation Qualifiers And Reason Codes to aggregate parameters (View/Edit)
21. Download Data For Offline Validation (Download)
22. Upload Offline Validated Data (Upload)
23. Best Result Findings (Review/Edit)
24. Validation Comments (Enter/Edit)
25. Validation Status Code (Change)
26. File With Validation Information (Download)
27. Miscellaneous Validation Reports (Display Report Options)
28. Run/Rerun Validation Checks
29. Do Not Validate This Dataset
30. Manual Validation Of This Dataset Is Complete
31. Change Validation Options Set
32. Send Notification That Validation Is Complete
33. Move All Validated Data Into Destination Tables

EIM Automated Data Review – Quality Control

Process EDD in Holding Table

Edit/Review Dataset

— *N3B-2025-2500_test.txt* (ID: *60900*) - *file format:* ***Analytical EDD (2025)***

Process | Delete | Validate

1. Summary Of Findings (View)
2. Sample Counts/Completeness Reports (Lab and Field Samples) (More)

MS/MSD Recoveries

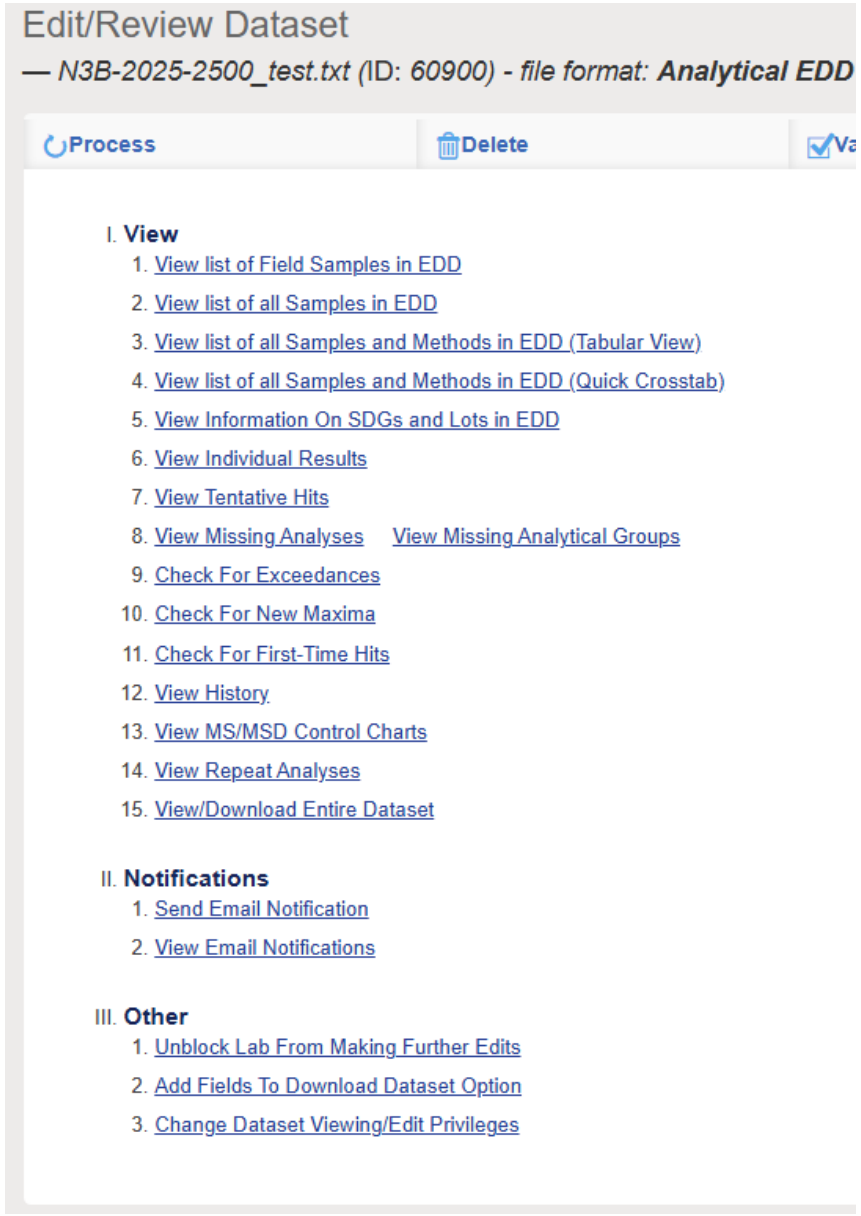
— *N3B-2025-2500_test.txt* (ID: *60900*)

Views

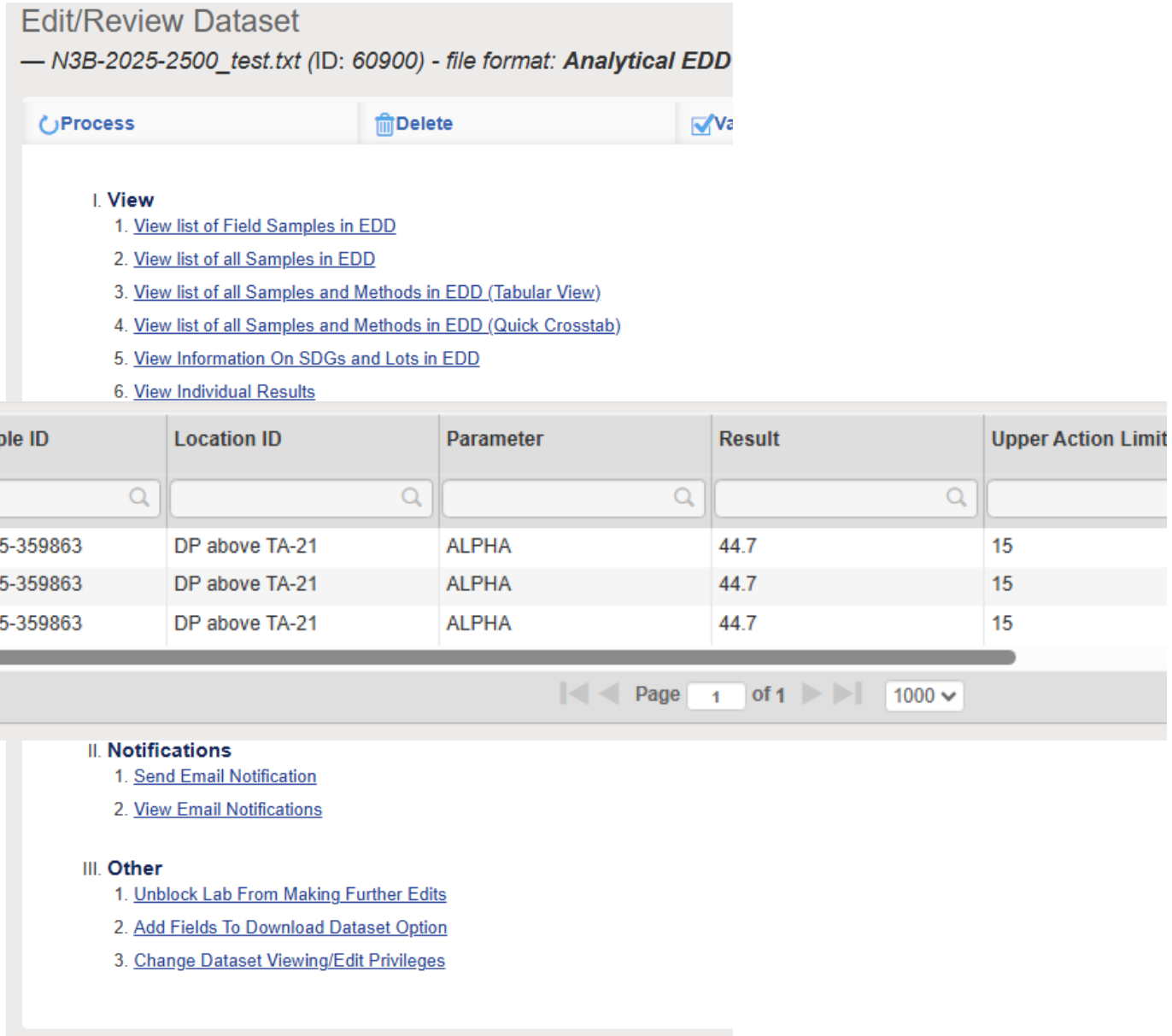
Lab Sample ID	Field Sample ID	FSID Dilution	FSID Field Prep	Spike Field Sample ID	Spike Dilution	Spike Field Prep	Spike Sample ID	Spike Dup Sample ID	Spike Type	Analytical Method	Parameter Name	Analysis Lot ID	Analysis Date	Sample Matrix	Spike % Recovery	Spike Dup % Recovery	Spike Upper % Limit	Spik Lowe Limit
730688001	WT_LAP-25-359855	1.00	UF	WT_LAP-25-359451	1.00	UF	1206156776		MS	EPA:310.1	Alkalinity-CO3+HCO3	2822481	07/01/2025	W	107		120	80
730688002	WT_LAP-25-359856	1.00	F	WT_LAP-25-359856	1.00	F	1206154099		PS	EPA:415.1	Dissolved Organic Carbon	2820919	06/28/2025	W	89.8		120	65
730688004	WT_LAP-25-359859	1.00	UF	WT_LAP-25-359859	1.00	UF	1206169117		MS	EPA:245.2	Mercury	2829792	07/17/2025	W	108		125	75
730688008	WT_LAP-25-359863	1.00	UF	WT_LAP-25-359863	1.00	UF	1206154409	1206154410	MS	EPA:900.0	Gross alpha	2821117	07/07/2025	W	104	109	125	75
730688009	WT_LAP-25-359864	1.00	UF	WT_LAP-25-360411	1.00	UF	1206158613	1206158614	MS	SW-846:8082A	Aroclor-1016	2823659	07/08/2025	W	69	62	107	38
730688009	WT_LAP-25-359864	1.00	UF	WT_LAP-25-360411	1.00	UF	1206158613	1206158614	MS	SW-846:8082A	Aroclor-1260	2823659	07/08/2025	W	48	42	114	37

22. Upload Offline Validated Data (Upload)
23. Best Result Findings (Review/Edit)
24. Validation Comments (Enter/Edit)
25. Validation Status Code (Change)
26. File With Validation Information (Download)
27. Miscellaneous Validation Reports (Display Report Options)
28. Run/Rerun Validation Checks
29. Do Not Validate This Dataset
30. Manual Validation Of This Dataset Is Complete
31. Change Validation Options Set
32. Send Notification That Validation Is Complete
33. Move All Validated Data Into Destination Tables

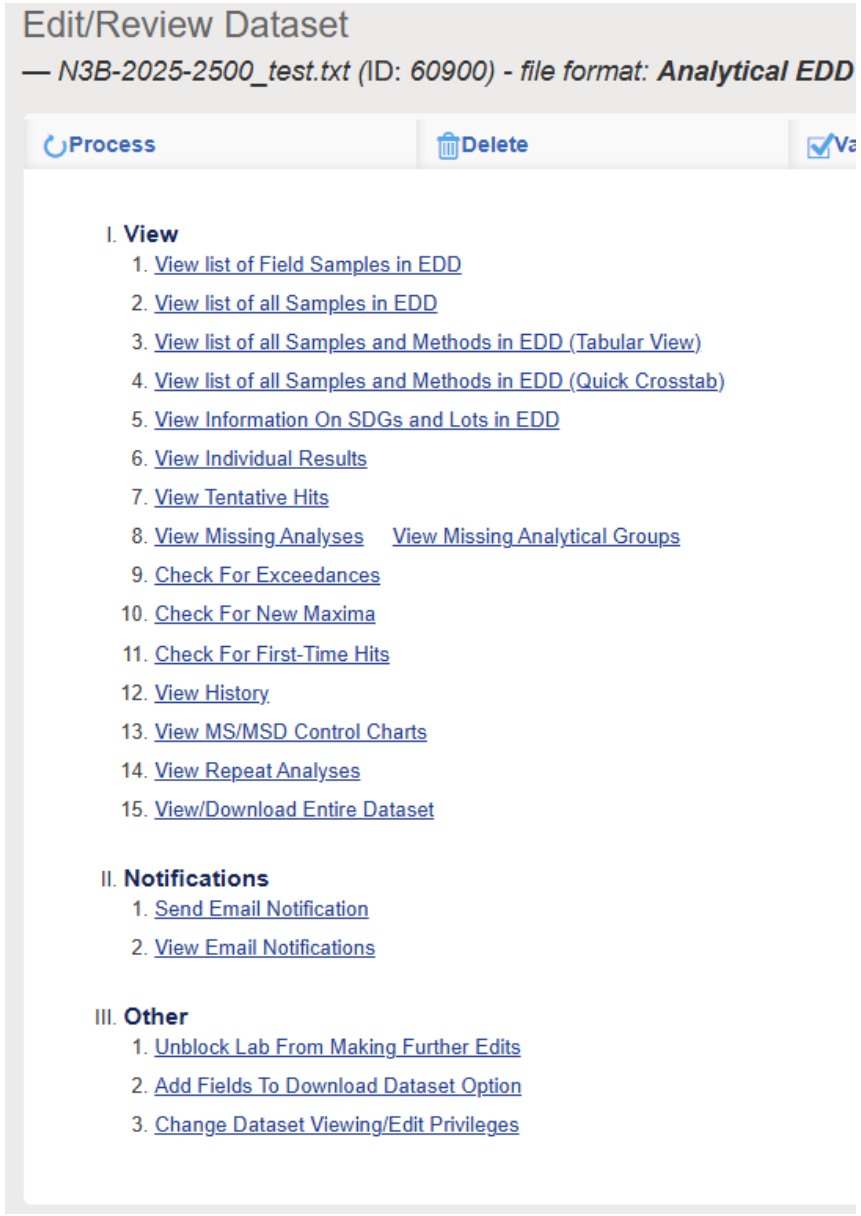
EIM Automated Data Review– Historical Data



EIM Automated Data Review– Historical Data



EIM Automated Data Review – Historical Data



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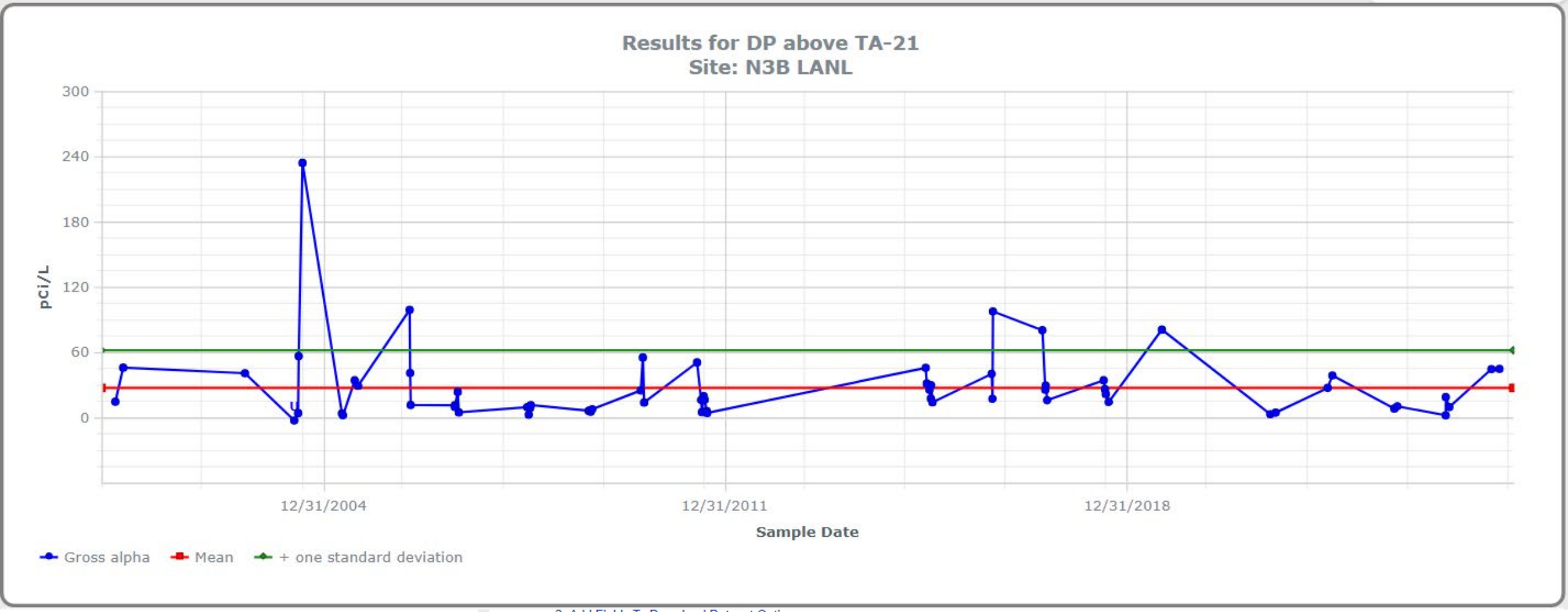
EIM Automated Data Review – Historical Data

Edit/Review Dataset

— N3B-2025-2500_test.txt (ID: 60900) - file format: **Analytical EDD**



2. Add Fields To Download Dataset Option
3. Change Dataset Viewing/Edit Privileges

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Automated Data Review Capabilities

- ADR can assist in the review and qualification of data based on the quality control that is reported in the electronic data deliverable:
  - Missing samples / analyses
  - Holding times
  - Missing QC
  - Method blank contamination
  - Laboratory control sample recovery
  - Surrogates recovery
  - Matrix spikes recovery
  - Duplicates (field and laboratory) precision
  - Tracer/carriers recovery

- ADR cannot review
  - Raw data
  - Preparation logs
  - Instrument logs
  - Standards
  - Initial calibrations
  - Calibration checks
  - Data package completeness
  - Internal standards (in some cases)

Automated Data Review Report

AUTOMATED DATA REVIEW SUMMARY REPORT

Chain Of Custody No. N3B-2024-3904

1. Distribution Of Samples In EDD.

SDG	Analytical Method	Regular Samples	Field Duplicates	Trip Blanks	Field Blanks	Equipment Blanks
675395	EPA:170.0	6	1	1		
675395	EPA:353.2					
675395	EPA:901.1	6	1			
675395	HASL-300:AM-241	6	1			
675395	HASL-300:ISOPU	6	1			
675395	HASL-300:ISOU	6	1			
675395	SM:A2340B					
675395	SW-846:6010D	6	1			
675395	SW-846:6020B	6	1			
675395	SW-846:6850	6	1			
675395	SW-846:7470A					
675395	SW-846:7471B	6	1			
675395	SW-846:8082A	2				
675395	SW-846:8260D	5		1		
675395	SW-846:8270E	6	1			
675395	SW-846:8330B	6	1			
675395	SW-846:9012B	6	1			
675395	SW-846:9045D	6	1			
675395	SW-846:9056A	6	1			

SDG	Analytical Method	Analysis Lot ID	Prep Lot ID	Regular Samples	Field Duplicates	Trip Blanks	Field Blanks	Equipment Blanks	Method Blanks	Matrix Spikes	Matrix Spike Dups	Analytical Spikes	Post-Digestion Spikes	Lab Control Samples	Lab Control Sample Dups	Blank Spike	Blank Spike Dups	Lab Duplicates	Storage Blanks	Preparation Blanks	Reagent Blanks
675395	EPA:170.0	NA	NA	6	1	1															
675395	EPA:353.2	2640162	2640162						1					1				1			
675395	EPA:901.1	2641921	2641921	6	1				1					1				1			
675395	HASL-300:AM-241	2640226	2640226	6	1				1					1				1			

Automated Data Review Report

AUTOMATED DATA REVIEW SUMMARY REPORT

Field Sample ID	Blank Lab Sample	Blank Type	Analytical Method	Parameter Name	Blank Lab Result	Blank Lab Units	Lab Result	Lab Qualifier	Lab Detection Limit	Detect Flag	Detect to Nondetect Factor	Detect to Estimated Factor	Use Factors
RE27-24-309655	1205788655	METHOD BLANK	SW-846:7471B	Mercury	-7.47	ug/kg	7.75	U	23.1	N	5	100	Y
RE27-24-309832	1205788655	METHOD BLANK	SW-846:7471B	Mercury	-7.47	ug/kg	7.10	U	21.2	N	5	100	Y
RE27-24-309620	675395007	TRIP BLANK	SW-846:8260D	Methylene Chloride	3.33	ug/kg	2.89	BJ	4.48	Y	10	100	Y
RE27-24-309620	1205792067	METHOD BLANK	SW-846:8260D	Methylene Chloride	3.29	ug/kg	2.89	BJ	4.48	Y	10	100	Y
RE27-24-309621	675395007	TRIP BLANK	SW-846:8260D	Methylene Chloride	3.33	ug/kg	3.26	BJ	4.51	Y	10	100	Y
RE27-24-309621	1205792067	METHOD BLANK	SW-846:8260D	Methylene Chloride	3.29	ug/kg	3.26	BJ	4.51	Y	10	100	Y
RE27-24-309632	675395007	TRIP BLANK	SW-846:8260D	Methylene Chloride	3.33	ug/kg	2.95	BJ	4.50	Y	10	100	Y
RE27-24-309632	1205792067	METHOD BLANK	SW-846:8260D	Methylene Chloride	3.29	ug/kg	2.95	BJ	4.50	Y	10	100	Y
RE27-24-309652	675395007	TRIP BLANK	SW-846:8260D	Methylene Chloride	3.33	ug/kg	3.07	BJ	4.87	Y	10	100	Y
RE27-24-309652	1205792067	METHOD BLANK	SW-846:8260D	Methylene Chloride	3.29	ug/kg	3.07	BJ	4.87	Y	10	100	Y
RE27-24-309655	675395007	TRIP BLANK	SW-846:8260D	Methylene Chloride	3.33	ug/kg	2.90	BJ	4.82	Y	10	100	Y
RE27-24-309655	1205792067	METHOD BLANK	SW-846:8260D	Methylene Chloride	3.29	ug/kg	2.90	BJ	4.82	Y	10	100	Y

Level 3 Validation Tracking

Manual Validation Tracking

View Results

— *Only pending EDDs for 2025*

Options

NOTES

EDD Filename	Sampling Program	Sample Matrix	Lab ID	D/F	Gen Chem	Gen Chem PC	HE	LC	Metals	Nitr...	PCB Con...	Per...	Pest...	PFAS	Rad Alpha	Rad Ga...	Rad Gen	Rad Matrix Spike	Rad Yield	SVOC	TPH	VOC	Validator	Validation Date	Reason
																									suspicious p-nitrotoluene new max at R-48
N3B-2025-2892.TXT	CO-GW	W	SWRI							S															
N3B-2025-2960.txt	CO-GW	W	GELC		S	S	T	S	T			S										S			Aluminum exceedance and new maxima, RDX exceedances and new maxima
N3B-2025-2789.TXT	NPDES-IP	W	SWRI			S																			
N3B-2025-2949.txt	CO-GW	W	GELC		O	O	T	O	O			O										O			RDX new max R-25b
N3B-2025-2948.txt	CO-Cr	W	GELC		S	S			S			S													
N3B-2025-2888.txt	CO-GW	W	GELC		X	X	X		X			X	X	X	S	S	S		S	X		X	cwhite	09/04/2025, 10/01/2025	FS does not match
N3B-2025-2880.txt	CO-GW	W	GELC		O	O	O		O			O	T	O	O	O	O	O	O	O		T			Hexachlorobenzene first time detection, o-Xylene first time detection
N3B-2025-2857.txt	CO-GW	W	GELC		O	O	O		T			O	O		O	O	O	O	O	O		O			Nickel New Maxima and Exceedances
N3B-2025-2755.txt	CO-Cr	W	GELC		T	T		S	T			S													Al det in filtered sample
N3B-2025-2718.txt	CO-GW	W	GELC		T	S			S			S		S	X	X	X		X				garrettj	09/08/2025, 09/15/2025	first time cyanide detection
N3B-2025-2677.txt	CO-GW	W	GELC		T	S		S	S			S								S			hwestbrook	09/18/2025	Total P new max

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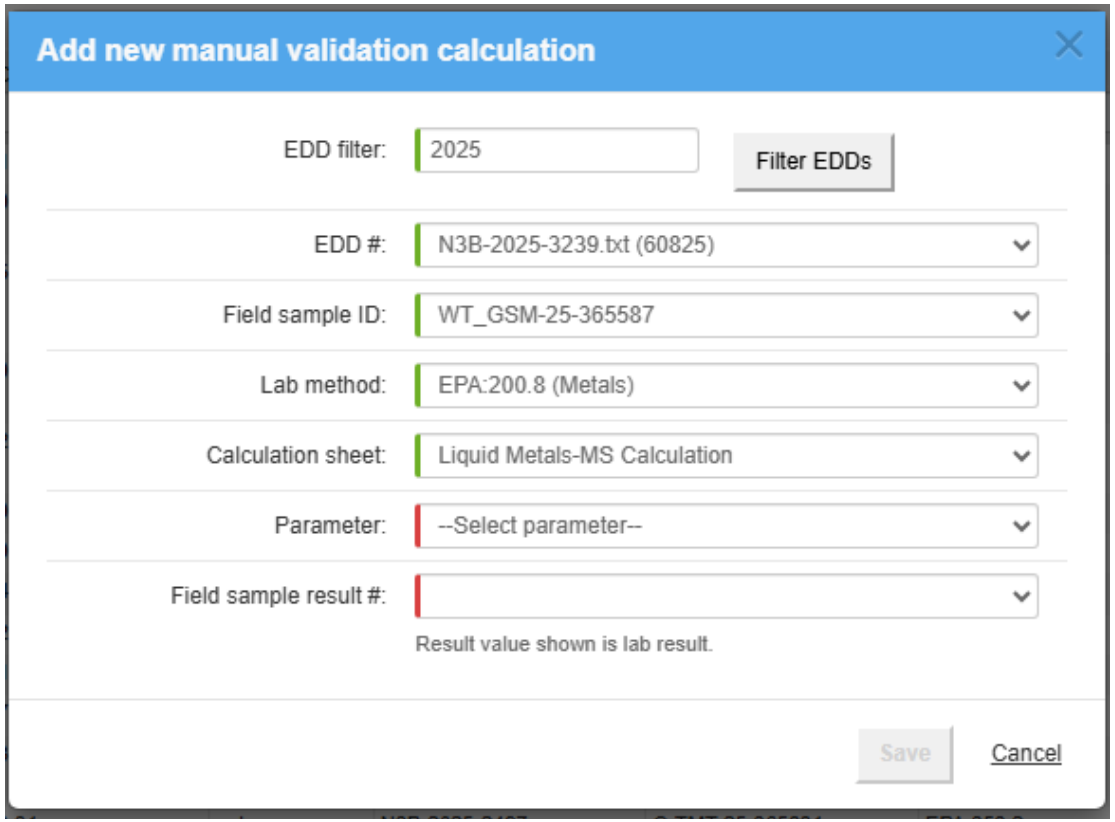
Level 3 Validation – Manual Calculation



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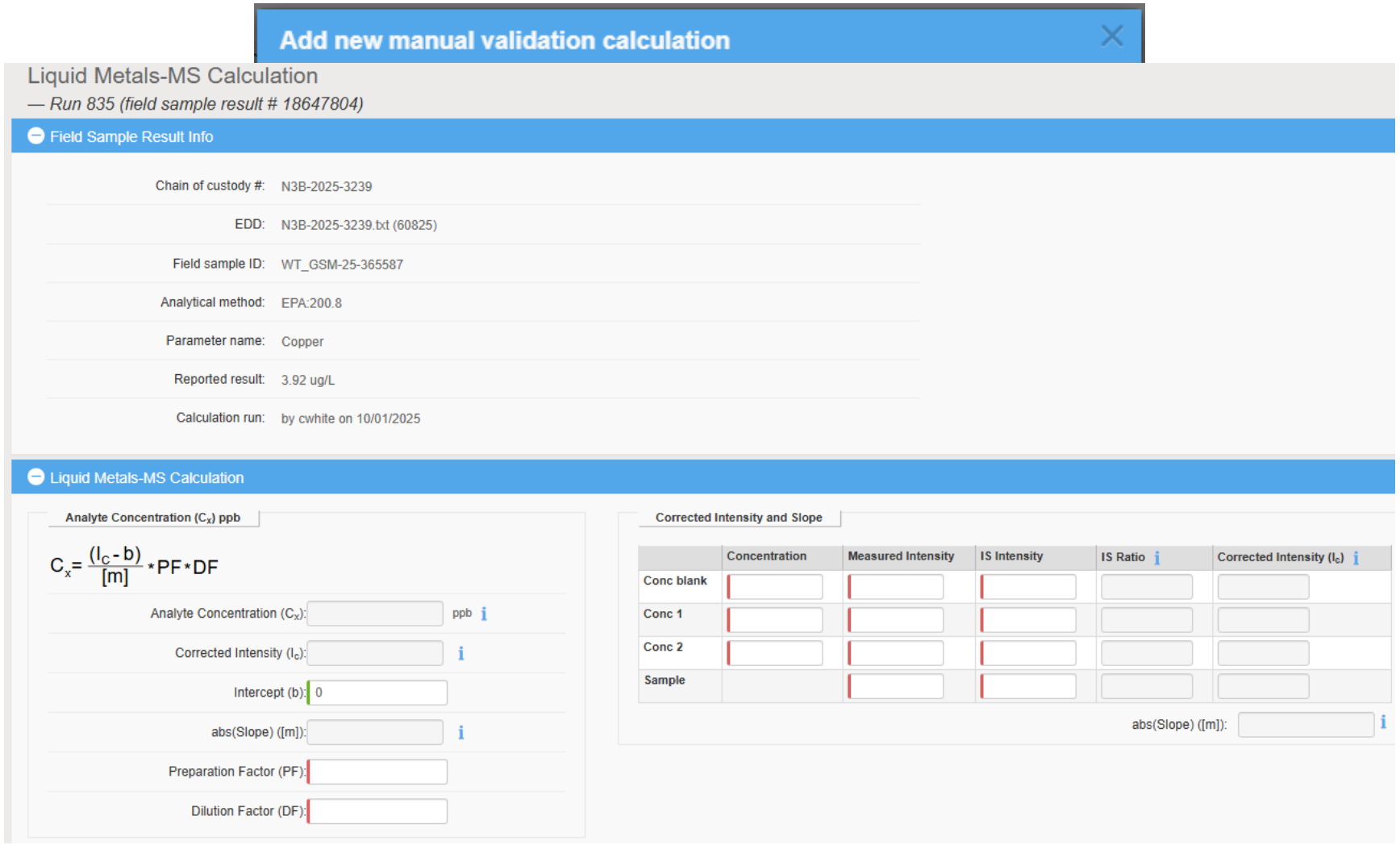
Level 3 Validation – Manual Calculation



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Level 3 Validation Report

N3B-Form-6046

Data Validation Report

Section I. General Information

COC: N3B-2024-3904 **Validation Date:** 09/26/2024 **SDG:** 675395

Contract Laboratory: GEL Laboratories, LLC

Project: FY24 Lower Pajarito Canyon SWMU 27-002 **Project Code:** CO-lPaj **Send To:**

Analytical Suite (Check All That Apply):

☒ **N3B-AP-SDM-3001**, *Validation of Volatile Organic Compounds Analytical Data*	☒ **N3B-AP-SDM-3002**, *Validation of Semivolatile Organic Compounds Analytical Data*	☒ **N3B-AP-SDM-3003**, *Validation of Organochlorine Pesticides and Herbicides and Polychlorinated Biphenyls Analytical Data*	☒ **N3B-AP-SDM-3005**, *Validation of Metals Analytical Data*
☐ **N3B-AP-SDM-3006**, *Validation of Radiochemical Analytical Data*	☒ **N3B-AP-SDM-3007**, *Validation of General Chemistry Analytical Data*	☒ **N3B-AP-SDM-3008**, *Validation of High Explosives Analytical Data*	☐ **N3B-AP-SDM-3009**, *Validation of Analytical Data by High-Resolution Gas Chromatography/High-Resolution Mass Spectrometry*
☐ **N3B-AP-SDM-3011**, *Validation of Total Petroleum Hydrocarbons Gasoline Range Organics/Diesel Range Organics Analytical Data*	☒ **N3B-AP-SDM-3012**, *Validation of Analytical Data by Liquid Chromatography and Liquid Chromatography/Tandem Mass Spectrometry*	☐ **Other (Describe)**	

☒ **Scheduled Validation** *or* ☐ **Triggered Validation (Reason and Parameter(s)):** Scheduled to meet project DQOs

Level 3 Validation Report

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N3B-Form-6046

Data Validation Report

Field Sample ID	Method	Matrix	Sample Date	Location
RE27-24-309632	SW-846:6010D, SW-846:6020B, SW-846:6850, SW-846:7471B, SW-846:8260D, SW-846:8270E, SW-846:8330B, SW-846:9012B, SW-846:9045D, SW-846:9056A	S	07/10/2024 11:15	27-34 (2-3)
RE27-24-309652	SW-846:6010D, SW-846:6020B, SW-846:6850, SW-846:7471B, SW-846:8082A, SW-846:8260D, SW-846:8270E, SW-846:8330B, SW-846:9012B, SW-846:9045D, SW-846:9056A	S	07/10/2024 09:50	27-40 (4-5)
RE27-24-309655	SW-846:6010D, SW-846:6020B, SW-846:6850, SW-846:7471B, SW-846:8082A, SW-846:8260D, SW-846:8270E, SW-846:8330B, SW-846:9012B, SW-846:9045D, SW-846:9056A	S	07/10/2024 09:10	27-41 (4-5)
RE27-24-309832	SW-846:6010D, SW-846:6020B, SW-846:6850, SW-846:7471B, SW-846:8270E, SW-846:8330B, SW-846:9012B, SW-846:9045D, SW-846:9056A	S	07/10/2024 11:45	27-95 (0-1)
RE27-24-309890 (FTB)	SW-846:8260D	S	07/10/2024 08:45	27-41 (NA-)
RE27-24-309916 (FR)	EPA:353.2, SM:A2340B, SW-846:6010D, SW-846:6020B, SW-846:6850, SW-846:7470A, SW-846:9012B	W	07/10/2024 10:30	27-30 (NA-)
RE27-24-309946 (FD)	SW-846:6010D, SW-846:6020B, SW-846:6850, SW-846:7471B, SW-846:8270E, SW-846:8330B, SW-846:9012B, SW-846:9045D, SW-846:9056A	S	07/10/2024 11:45	27-95 (0-1)

Level 3 Validation Report

- Table of updates to be made in the EIM data base

Updates to EIM Qualifiers and/or Reason Codes

Location ID	Field Sample ID	Parameter Name	Report Result	Report Units	Existing Qualification		New Qualification	
					Validation Qualifier	Validation Reason Codes	Validation Qualifier	Validation Reason Codes
See Samples Table	RE27-24-309620 RE27-24-309621 RE27-24-309632 RE27-24-309652 RE27-24-309655 RE27-24-309832 RE27-24-309946	Tetryl	0.15 0.146 0.141 0.15 0.142 0.142 0.148	mg/kg	U	U_LAB	UJ	HE7c

Summary

- N3B data review processes have been set up to optimize quality and efficiency
- The assistance of the EIM Automated Data Review module allows N3B chemists to review large data sets in a timely manner without compromising quality
- Tools to help to optimize the process
  - Automated Data Review assists in identifying potential problems based on comparisons to historical data
  - Validation tracking ensures that a representative number of data sets are Level 3 validated
  - Manual calculations allow N3B chemists to quickly verify that the laboratory LIMS systems and other processes are working as expected to report out final data


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