Improving Quality, Efficiency, and Cost-Effectiveness of Data Validation through Increased Automation

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Presentation Overview

- Data Quality Assessment and Validation
  - Brief background
  - How can we improve?
- Example: Data Validation Project with Metrics
- Recommendations and Effect on
  - Quality
  - Efficiency
  - Cost-Effectiveness

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Data Quality Assessment and Validation

- Progress in automated data review through mid1990s – many labs delivered more QC elements in 1998 than they do today
- What stopped the progress?

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Data Quality Assessment and Validation

- What stopped the progress?
  - Counter intuitively – focus on standardization
  - 'Wait and See' attitude from providers concerned about choosing the wrong path
  - Contracting mechanisms associated with little incentive for 'better, faster, cheaper'

Presently, a combination of automated and manual procedures is used in the validation industry.

Can we increase the automation?

Data Quality Element	Manual	Electronic
Chain-of-Custody	x	
Condition Upon Receipt	x	
Case Narrative	x	
Holding Times		x
Sample Results		x
Field Blanks		x
Equipment Blanks		x
Trip Blanks		x
Field Duplicates or Replicates		x
Dilution Factors		x
Detection Limits		x
Quantitation Limits		x
Method Blanks		x
Laboratory Control Samples		x
Matrix Spike / Matrix Spike Duplicates		x
Laboratory Duplicates		x
Surrogates		x
Tracers or Labeled Analogs	x	
Post-Digestion Spikes	x	
Serial Dilutions	x	
Preparation Logs	x	
Instrument Logs	x	
Internal Standards	x	
Instrument Tunes	x	
Calibration Blanks	x	
Initial Calibrations	x	
Initial Calibration Verifications	x	
Continuing Calibration Verifications	x	
Sample Chromatograms	x	
Mass Spectra	x	
Raw Data	x	

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Example: Multi-Year DoD Remediation Project

- 450 soil samples during first phase
- 70,250 analytical results
- 100% review of data deliverables
  - Manual review of general information
  - Automated review of available electronic data
  - Manual review of
    - instrument calibration data
    - additional method QC data for metals and organics

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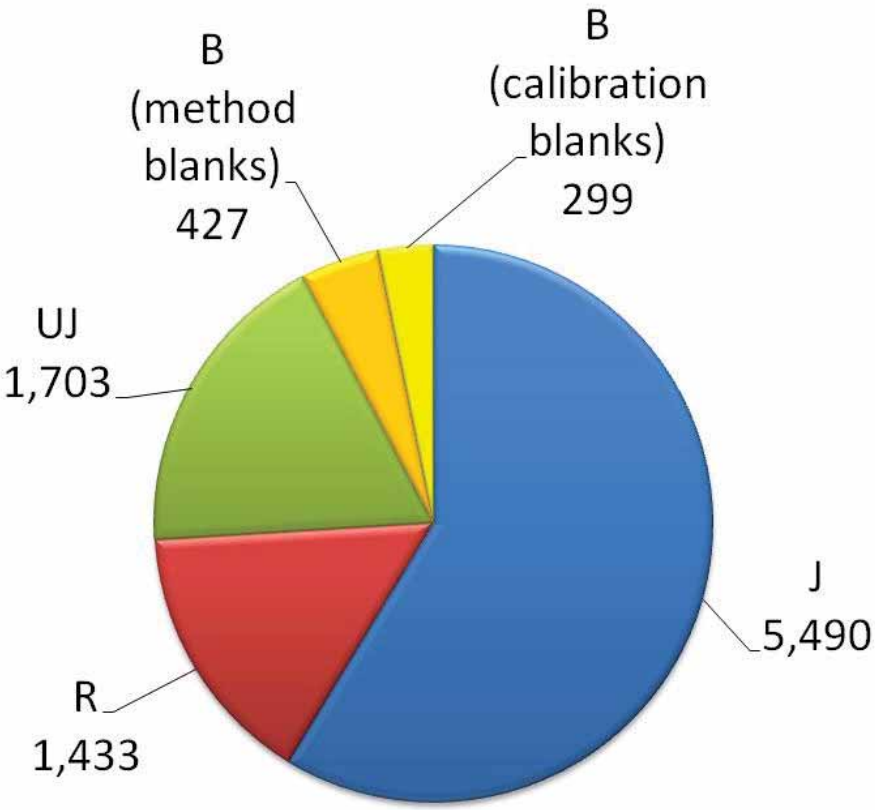
Of 70,250 results, 9352 results (13%) were qualified



Calibration Blanks – Metals

Analyte	Initial Calib. Blank (ug/L)	C	Continuing Calibration Blank (ug/L) 10	C	11	C	12	C	Prepa-ration Blank	C	M
Aluminum	10.000	U	10.000	U	41.100		7.600	J	0.541	J	P
Antimony	5.000	U	5.000	U	5.000	U	5.000	U	0.500	U	P
Arsenic	5.000	U	5.000	U	5.000	U	5.000	U	0.500	U	P
Barium	5.000	U	5.000	U	5.000	U	5.000	U	0.500	U	P
Beryllium	2.000	U	2.000	U	2.000	U	2.000	U	0.500	U	P
Cadmium	2.000	U	2.000	U	2.000	U	2.000	U	0.500	U	P
Chromium	5.000	U	5.000	U	5.000	U	5.000	U	0.500	U	P
Cobalt	5.000	U	5.000	U	5.000	U	5.000	U	0.500	U	P
Copper	5.000	U	5.000	U	5.000	U	5.000	U	0.500	U	P
Iron	200.000	U	200.000	U	71.100	J	200.000	U	50.000	U	P
Lead	5.000	U	5.000	U	0.780	J	5.000	U	0.054	J	P
Manganese	5.000	U	5.000	U	5.000	U	5.000	U	0.500	U	P
Molybdenum	5.000	U	5.000	U	5.000	U	5.000	U	0.500	U	P
Nickel	5.000	U	5.000	U	5.000	U	5.000	U	0.500	U	P
Selenium	-1.107		-0.840		-1.000		-1.300		0.500	U	P
Silver	5.000	U	5.000	U	5.000	U	5.000	U	0.500	U	P
Thallium	2.000	U	2.000	U	2.000	U	2.000	U	0.500	U	P
Vanadium	-2.543		[illegible]		[illegible]		[illegible]		[illegible]		
Zinc	5.000										

EPA Sample No.	D/F	Time	% R	Analytes AL	SB	AS	BA	BE	CD	CA	CR	CO	CU	FE	PB	MG	MN	HG	MO	NI	K	SE	AG	NA	SR	TL	SN	TI	V	ZN
ICB-11	1	1708	0	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X
ICV-11	1	1711	0	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X
[redacted] 1	1	1720	0		X	X		X	X		X	X	X		X				X	X		X	X			X			X	X
[redacted] 2	1	1725	0		X	X		X	X		X	X	X						X	X		X	X			X			X	X
[redacted] 3	1	1727	0		X	X		X	X		X	X	X		X				X	X		X	X			X			X	
[redacted] 4	1	1729	0		X	X		X	X		X	X	X		X				X	X		X	X			X			X	X
[redacted] 5	1	1732	0		X	X		X	X		X	X	X		X				X	X		X	X			X			X	X
ICB-12	1	1737	0	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X
ICV-12	1	1739	0	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X
ICB-13	1	1741	0	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X
ICV-13	1	1744	0	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X
ZZZZZZ	1	1746	0	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X
ZZZZZZ	1	1748	0	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X
CSA	1	1751	0	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X
CSAB	1	1753	0	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X

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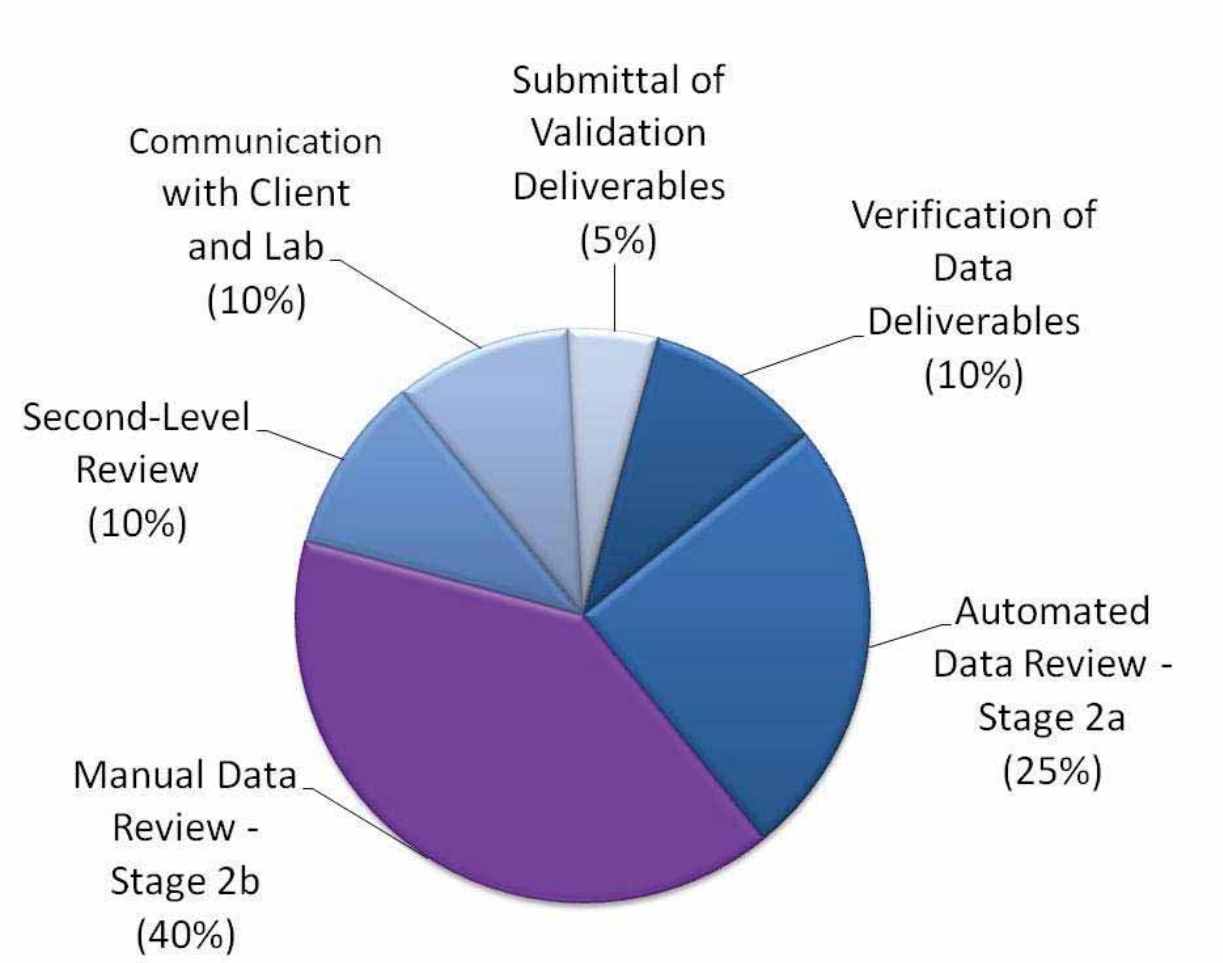
Percentage of Time Spent on Data Review and Validation Tasks



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What if even a subset of these numeric instrument QC elements could be assessed electronically?

Data Quality Element	Manual	Electronic
Chain-of-Custody	x	
Condition Upon Receipt	x	
Case Narrative	x	
Holding Times		x
Sample Results		x
Field Blanks		x
Equipment Blanks		x
Trip Blanks		x
Field Duplicates or Replicates		x
Dilution Factors		x
Detection Limits		x
Quantitation Limits		x
Method Blanks		x
Laboratory Control Samples		x
Matrix Spike / Matrix Spike Duplicates		x
Laboratory Duplicates		x
Surrogates		x
Tracers or Labeled Analogs	x	
Post-Digestion Spikes		x
Serial Dilutions		x
Preparation Logs	x	
Instrument Logs	x	
Internal Standards		x
Instrument Tunes	x	
Calibration Blanks		x
Initial Calibrations		x
Initial Calibration Verifications		x
Continuing Calibration Verifications		x
Sample Chromatograms	x	
Mass Spectra	x	
Raw Data	x	

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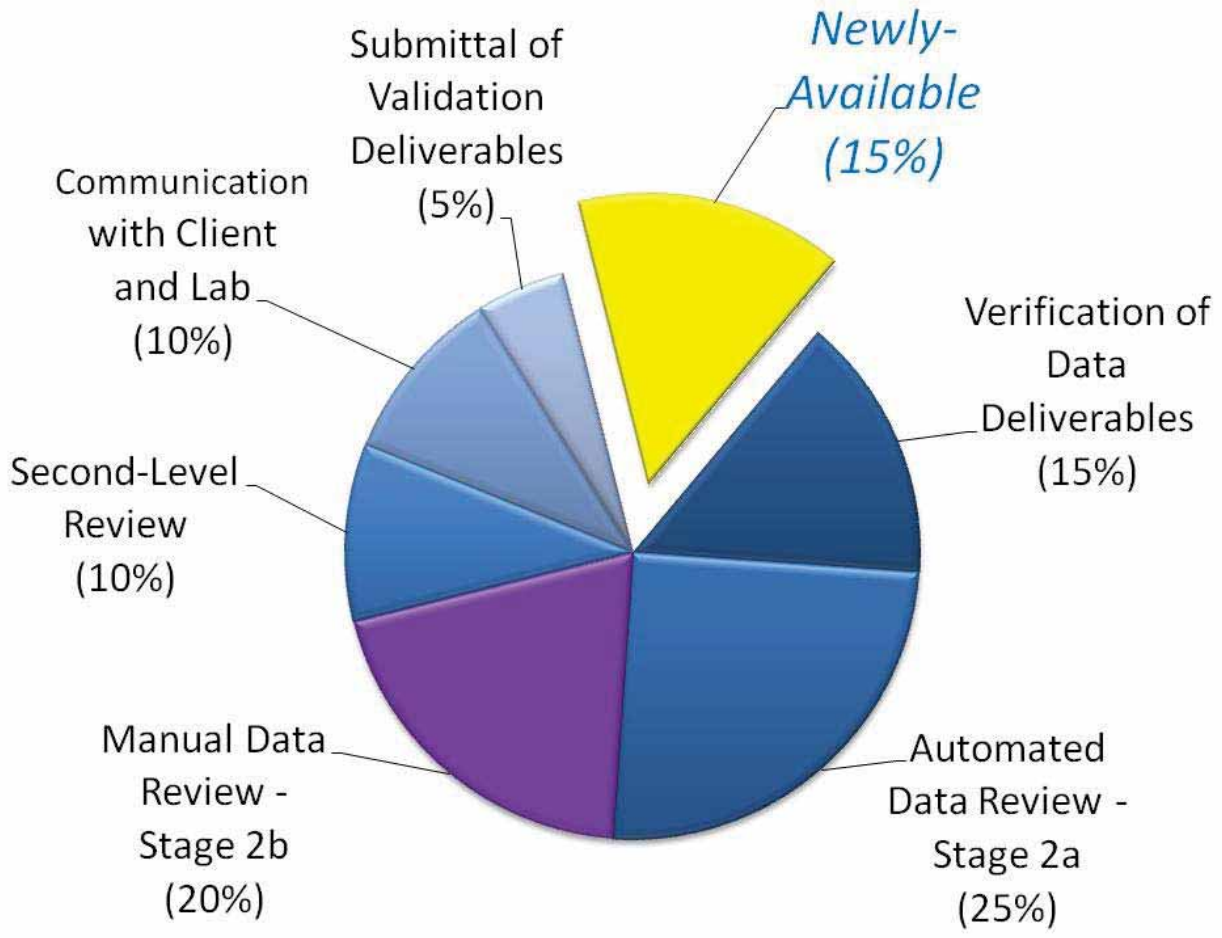
Estimated Percentage of Time with Enhanced Electronic Deliverables



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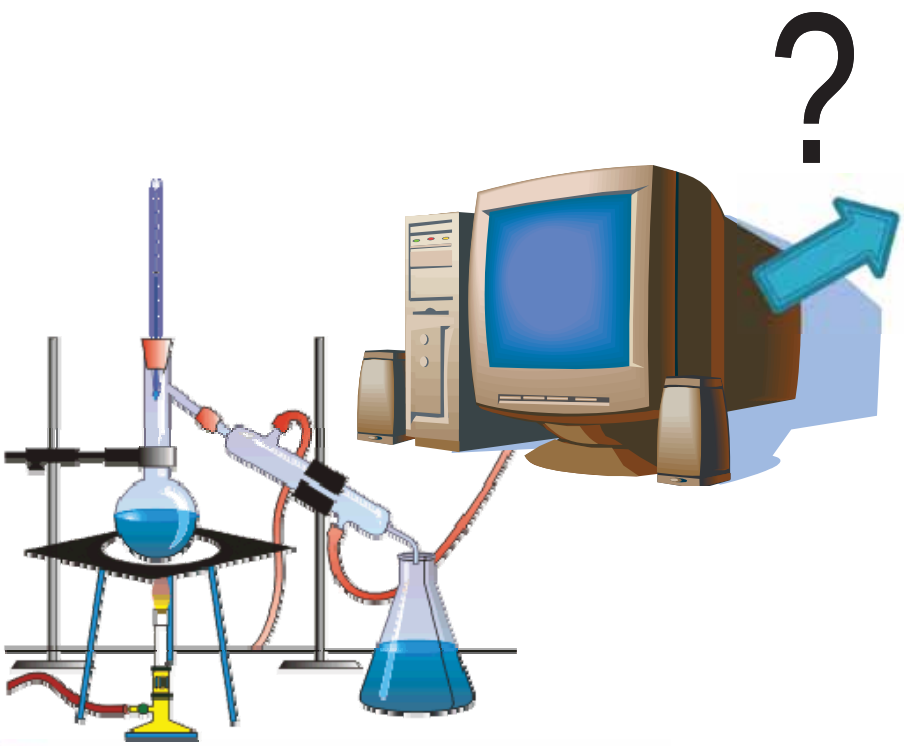
So if an increased level of automated review is a good thing, how do we get there?



Calibration | Soil | Water

Analyte Label	Analyte Name	ICAL RSD	ICAL Correlation Coefficient	ICV Lower Estimation	ICV Upper Estimation	CCV Lower Estimation	CCV Upper Estimation
630-20-6	1,1,1,2-TETRACHLOROETHANE	30.00	0.99	-20.00	20.00	-20.00	20.00
71-55-6	1,1,1-TRICHLOROETHANE	30.00	0.99	-20.00	20.00	-20.00	20.00
79-34-5	1,1,2,2-TETRACHLOROETHANE	30.00	0.99	-20.00	20.00	-20.00	20.00
79-00-5	1,1,2-TRICHLOROETHANE	30.00	0.99	-20.00	20.00	-20.00	20.00
76-13-1	1,1,2-Trifluoro-1,2,2-trichloroethane [Fr						
75-34-3	1,1-DICHLOROETHANE	30.00	0.99	-20.00	20.00	-20.00	20.00
75-35-4	1,1-DICHLOROETHENE	30.00	0.99	-20.00	20.00	-20.00	20.00
563-58-6	1,1-DICHLOROPROPENE	30.00	0.99	-20.00	20.00	-20.00	20.00
87-61-6	1,2,3-TRICHLOROBENZENE	30.00	0.99	-20.00	20.00	-20.00	20.00
96-18-4	1,2,3-TRICHLOROPROPANE	30.00	0.99	-20.00	20.00	-20.00	20.00
526-73-8	1,2,3-TRIMETHYLBENZENE						
120-82-1	1,2,4-TRICHLOROBENZENE	30.00	0.99	-20.00	20.00	-20.00	20.00
95-63-6	1,2,4-TRIMETHYLBENZENE	30.00	0.99	-20.00	20.00	-20.00	20.00
96-12-8	1,2-DIBROMO-3-CHLOROPROPANE	30.00	0.99	-20.00	20.00	-20.00	20.00
106-93-4	1,2-DIBROMOETHANE	30.00	0.99	-20.00	20.00	-20.00	20.00
95-50-1	1,2-DICHLOROBENZENE	30.00	0.99	-20.00	20.00	-20.00	20.00
107-06-2	1,2-DICHLOROETHANE	30.00	0.99	-20.00	20.00	-20.00	20.00
540-59-0	1,2-Dichloroethene						
78-87-5	1,2-DICHLOROPROPANE	30.00	0.99	-20.00	20.00	-20.00	20.00
354-23-4	1,2-Dichlorotrifluoroethane [Freon 123a						

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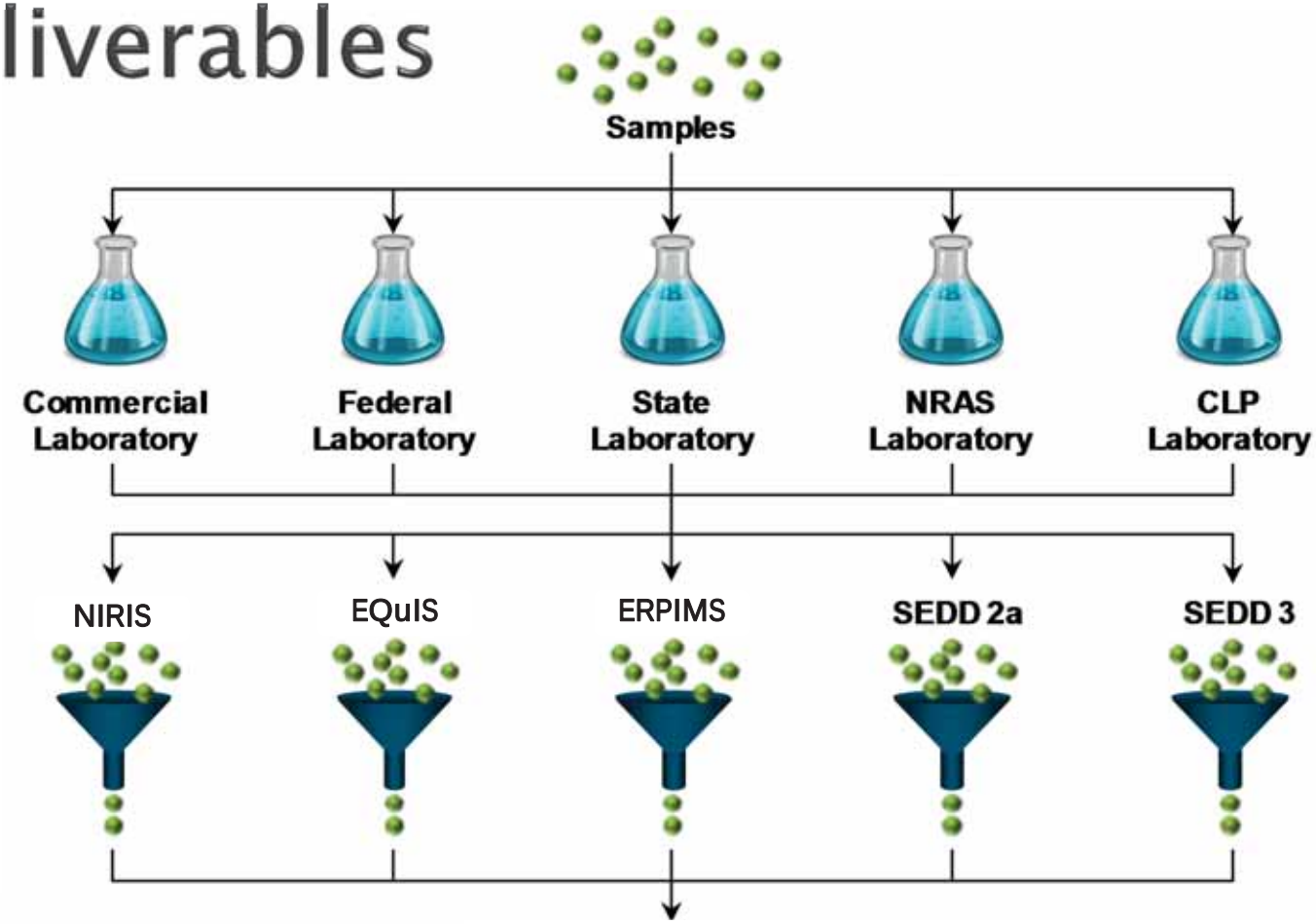
Currently, labs produce over 100 different types of electronic deliverables



Slide courtesy of
Sara Goehl, U.S. EPA

Isn't One Format the Answer?

"Absolutely! As long as it's ours!"

- -Everyone

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If Standardizing Isn't Happening…

- Laboratories now have IT tools in place to provide a wide range of EDDs
- EDD formats received from the lab are related to final deliverables only in terms of content
  - Work with your laboratories to obtain additional quality control elements in the format that works with your data management and Automated Data Review systems
  - Export validated data to your government clients in their required format

The Result…..?

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Improvements in the Inter-related Components of Quality, Efficiency, and Cost-Effectiveness

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Improvements in *Quality*

- Reduces potential for data validator errors
  - Less chance of manually entering an incorrect qualifier
  - Less likely to overlook items that require data qualification
- Allows for more consistent evaluation
  - By single validator over extended project
  - By multiple validators involved in single project

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Gains in *Efficiency*

- Can quickly and easily evaluate entire data set rather than a subset
- Can involve lower-level staff to a greater extent

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Greater *Cost-Effectiveness*

- Based on the example used in this presentation, validation costs could be reduced by an estimated 15% or more
- Reduced manual review time results in shortened turnaround times for validation deliverables and, thus, for project decision-making

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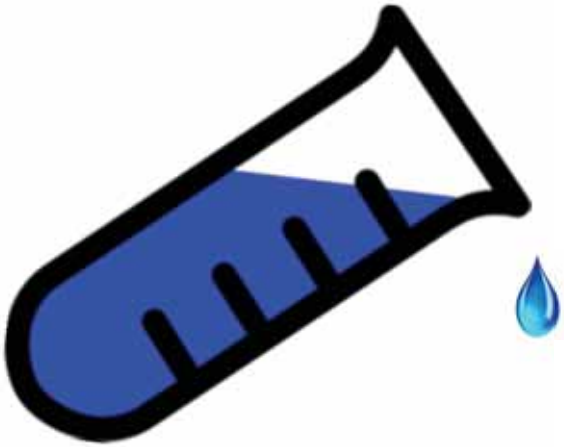
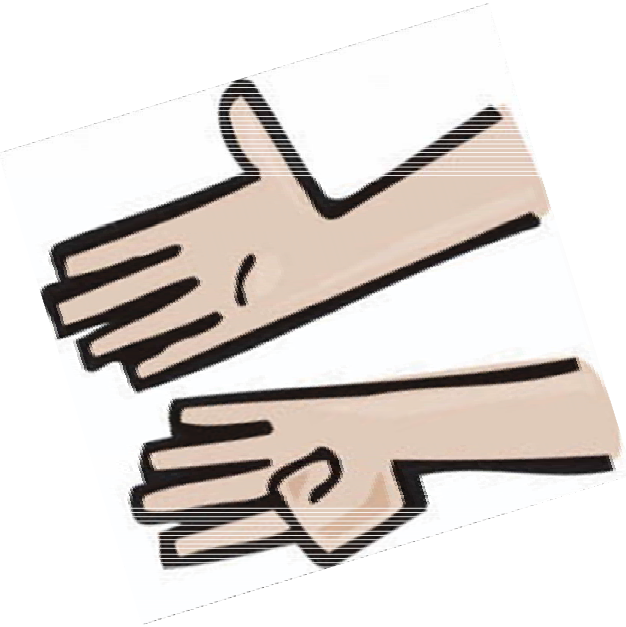
Ask the lab what they can do…and we'll do our part to make it work!





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Thank you! Questions?

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