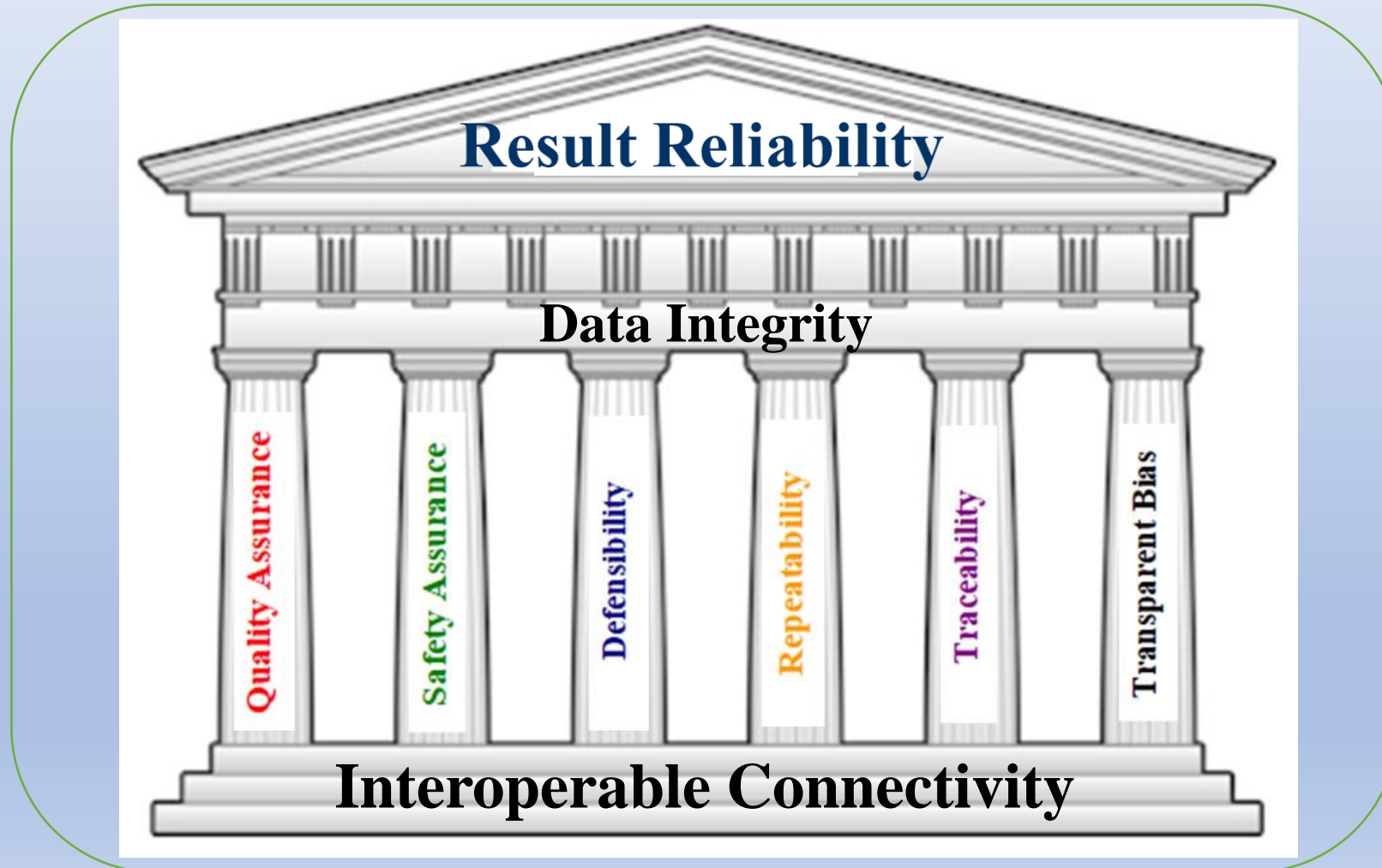


The Pillars of Data Integrity in Laboratory Data Automation



AGENDA: Data Integrity Automation

- Overview: Establishing the Components of Data Integrity
 - Importance of Result Reliability
 - When Results are Un-Reliable
 - Data Process Gaps in Lab Data Life Cycle
 - What are the Pain Points Inside the lab?
 - Pillars of Result Reliability for 100% Data Integrity
- Solutions
 - Automation and 100% Data Integrity
 - Quality Assurance (QC Samples)
 - Safety Assurance (Field Samples)
 - Defensibility, Repeatability, Traceability, and Transparent Bias
 - Early Notifications and Control Centers
- Use Case – LCMS PFAS Analysis to UCMR

Importance of Result Reliability



Sound Decisions



Immediate Impact on Health



Long Term Impact on Health



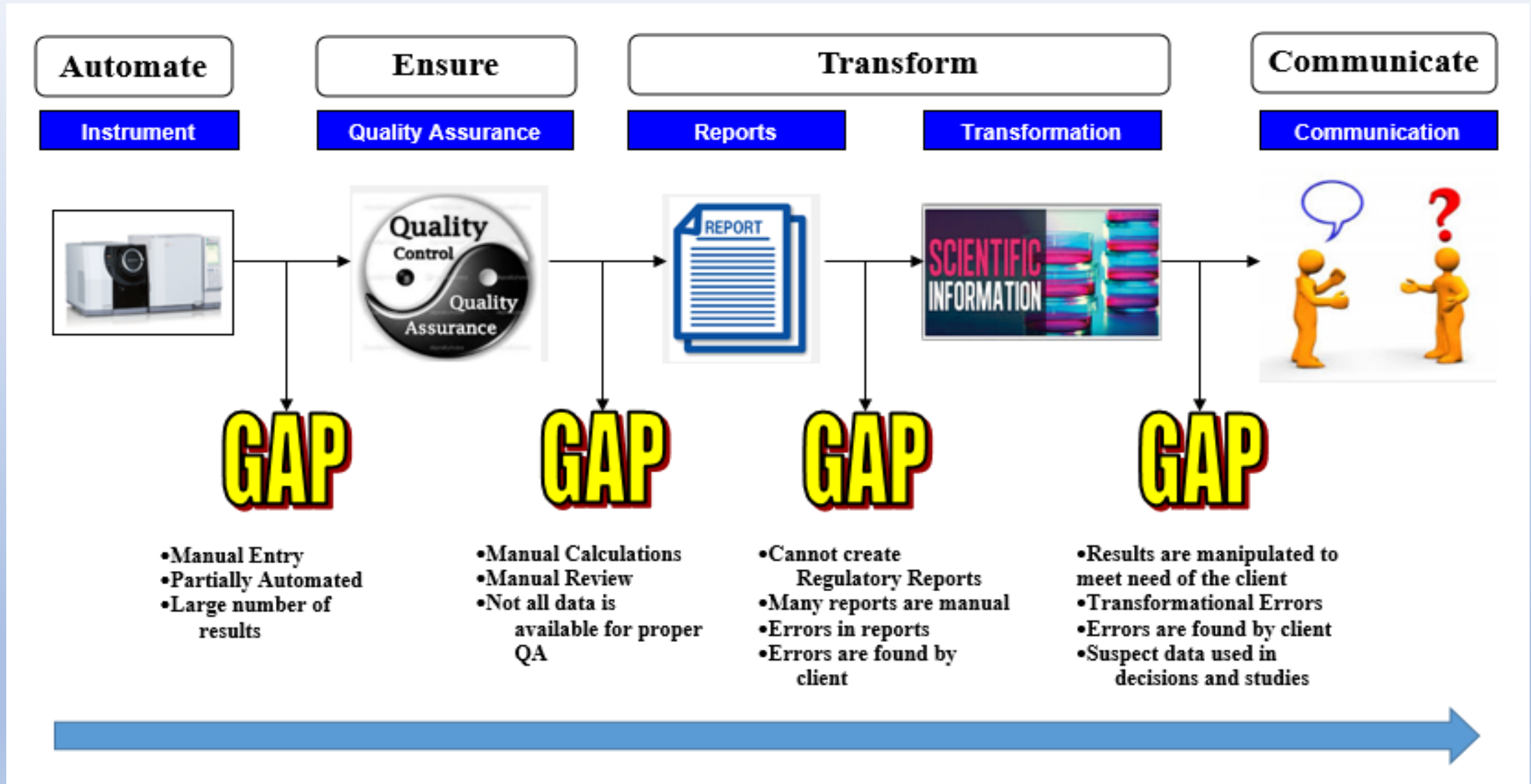
Impact On Where We Live



Future Impact

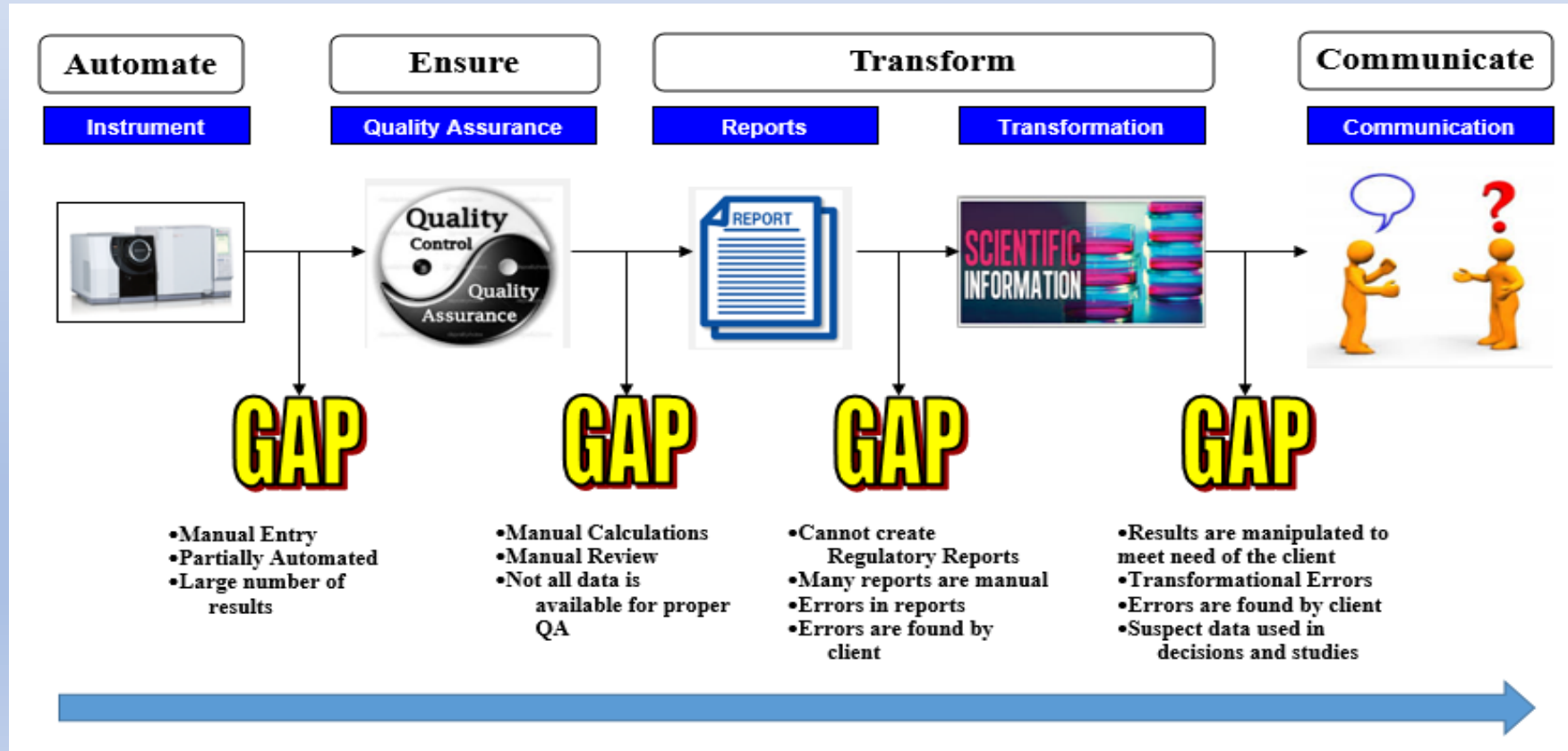
Did I Learn About Lab Data Integrity in Kindergarten?..





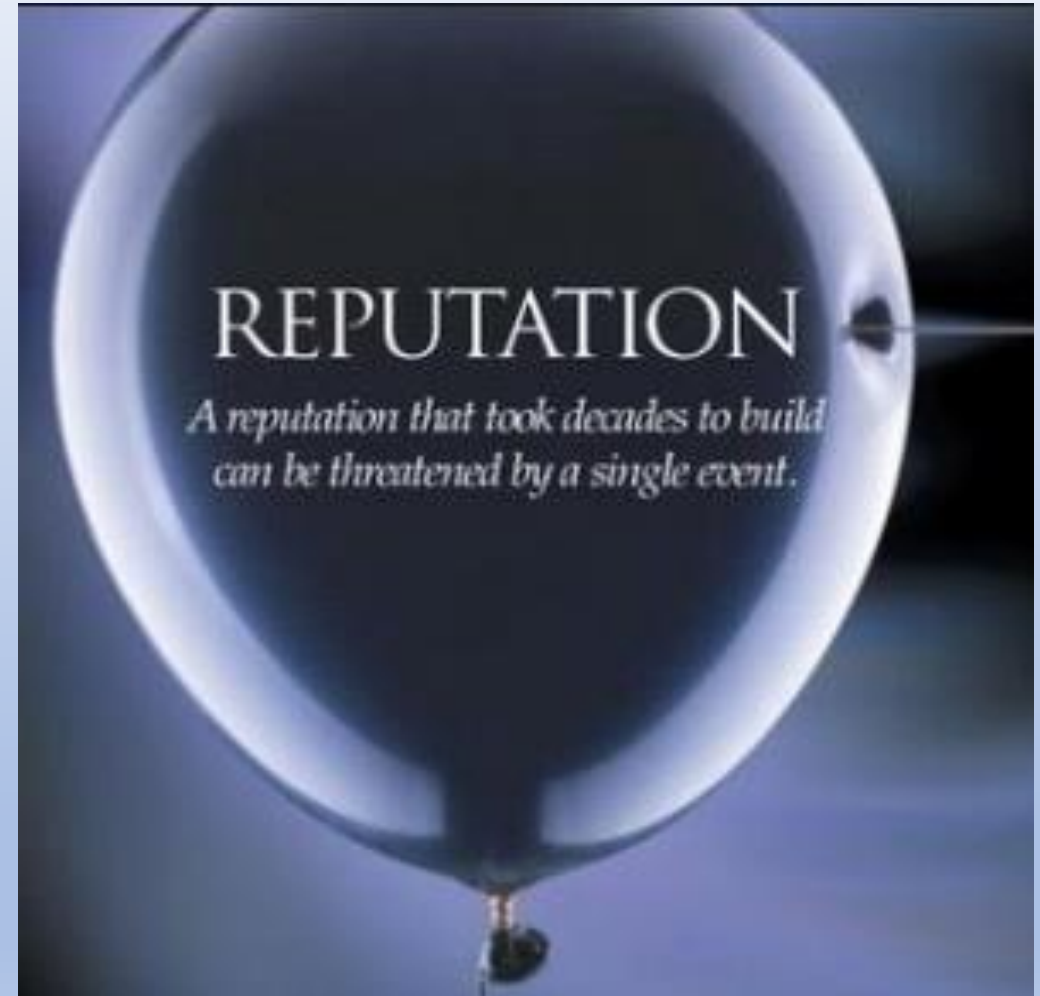
Problem: What & Where are the Gaps?

- Manual and Duplicate Data Entry
- Disparate Data Sources
- LIMS/IMS/3rd Party Connection
- Manual Quality Assurance Process
- Data “Gymnastics” for Connectivity at Data Points of Transfer

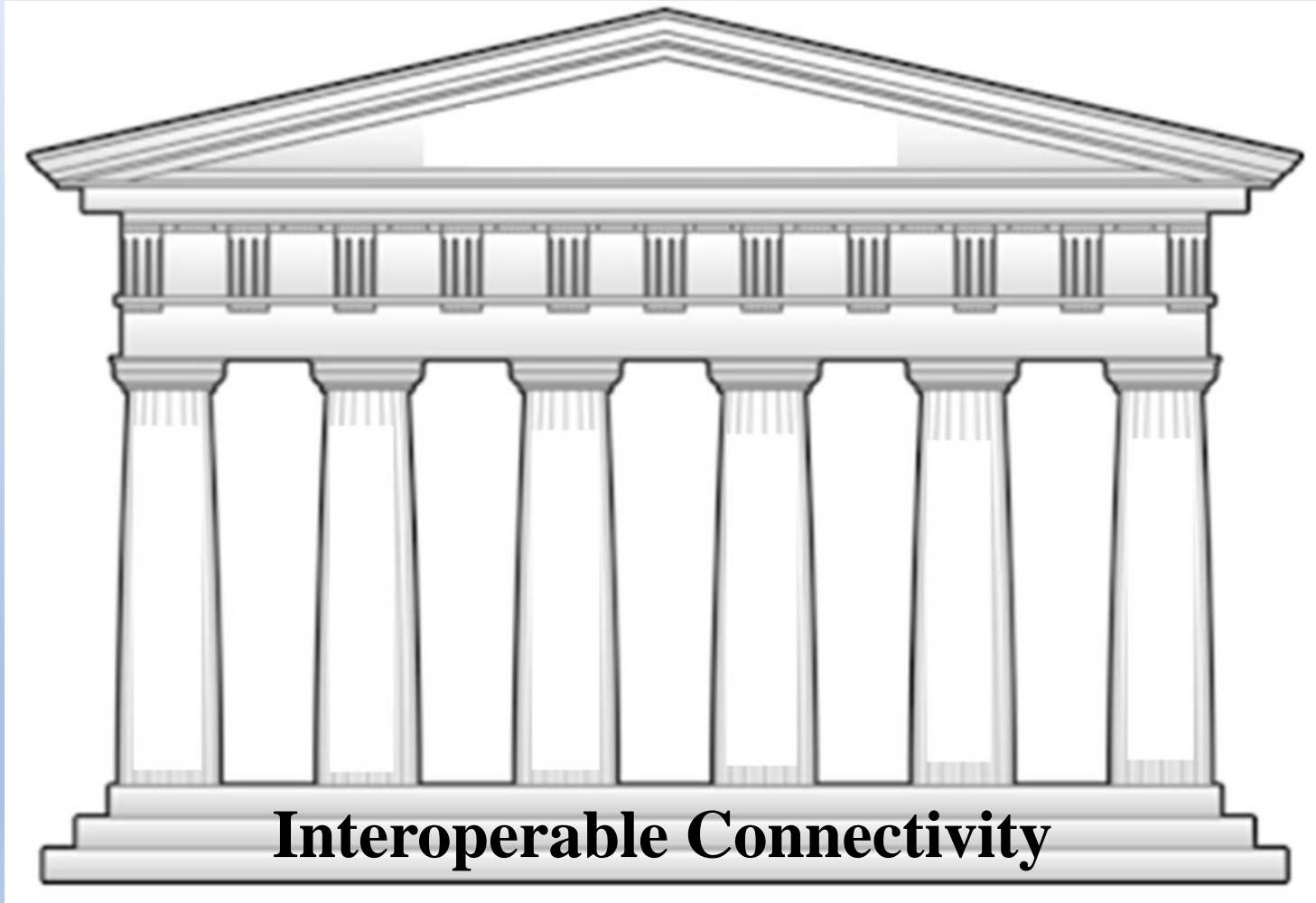


Data Integrity Effects All of Us

- Falsifying Tune and Calibration samples on hazardous material analysis.
- Changing performance results to show low emissions.
- Toxic metals found in drinking water not revealed.
- Hazardous decisions due to data manipulation and no peer review.

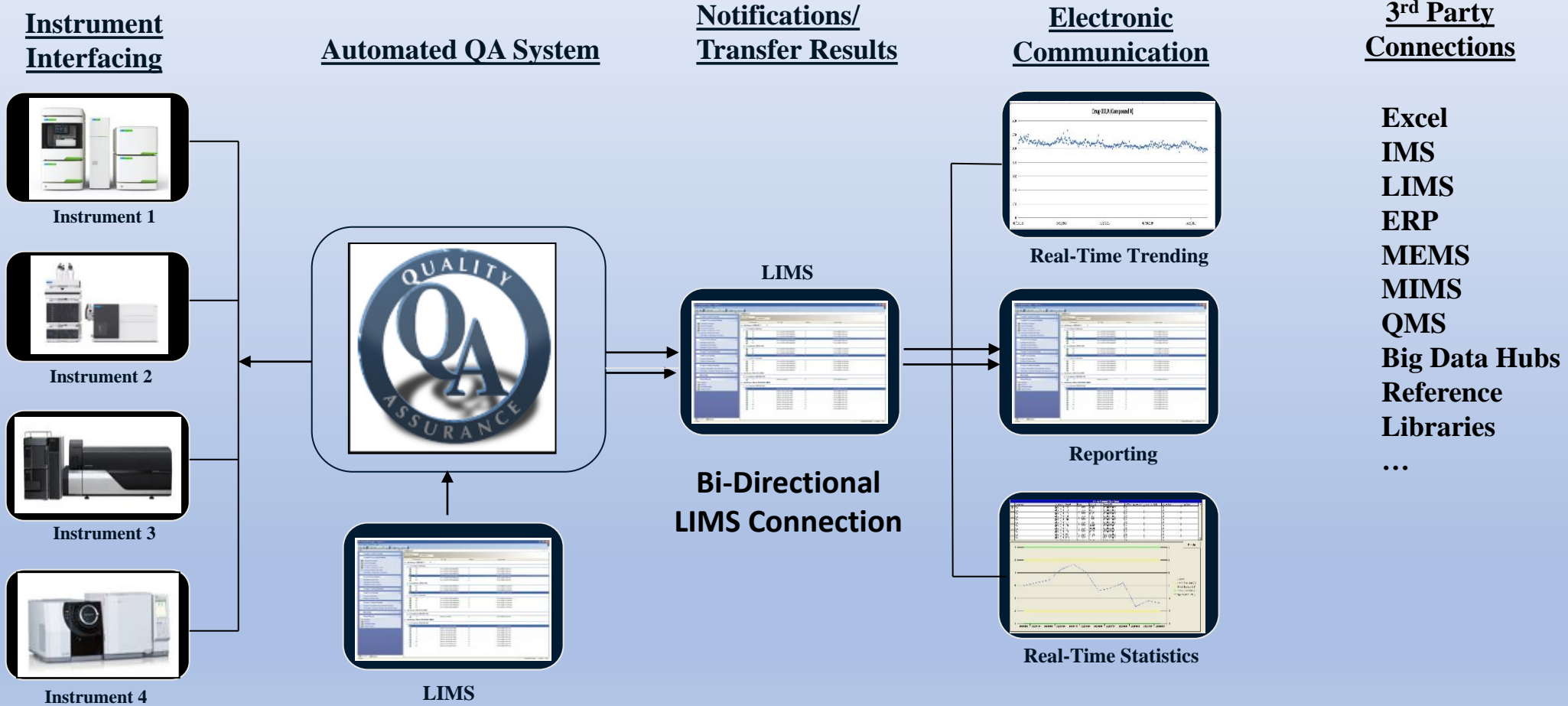


Pillars of Result Reliability: 100% Data Integrity



Automation Solutions for Functionality Gaps – Enhancing the Lab’s Present Process

Interoperable Connectivity



Pillars of Automated Data Integrity: Automated Quality Assurance



- All Quality Control
 - Field
 - Sampling
 - Instrument
 - Preparation
 - Sample Parameter QC
- Association of QC
- Communication of QC Exceedance

Priority Order of Analytical Review – Method, Client, Regulatory, Reporting



Instrument QC
Preparation QC
Sample Parameter QC – ISTD and Surrogates
QC Failure Associations to Target Samples
Over Linear Range
Reruns and Dilutions

Client Requirements

Regulatory Requirements

Reporting Requirements

QAP - Analytical Review and Approval

Reliable and Qualified Reportable Results

Key Batch Associations



Analytical Batch Example

- Tune
- Initial Calibrations

- Continuing Calibration Verification
- Method Blank/Negative Control
- Laboratory Control Sample
- Positive Control Sample

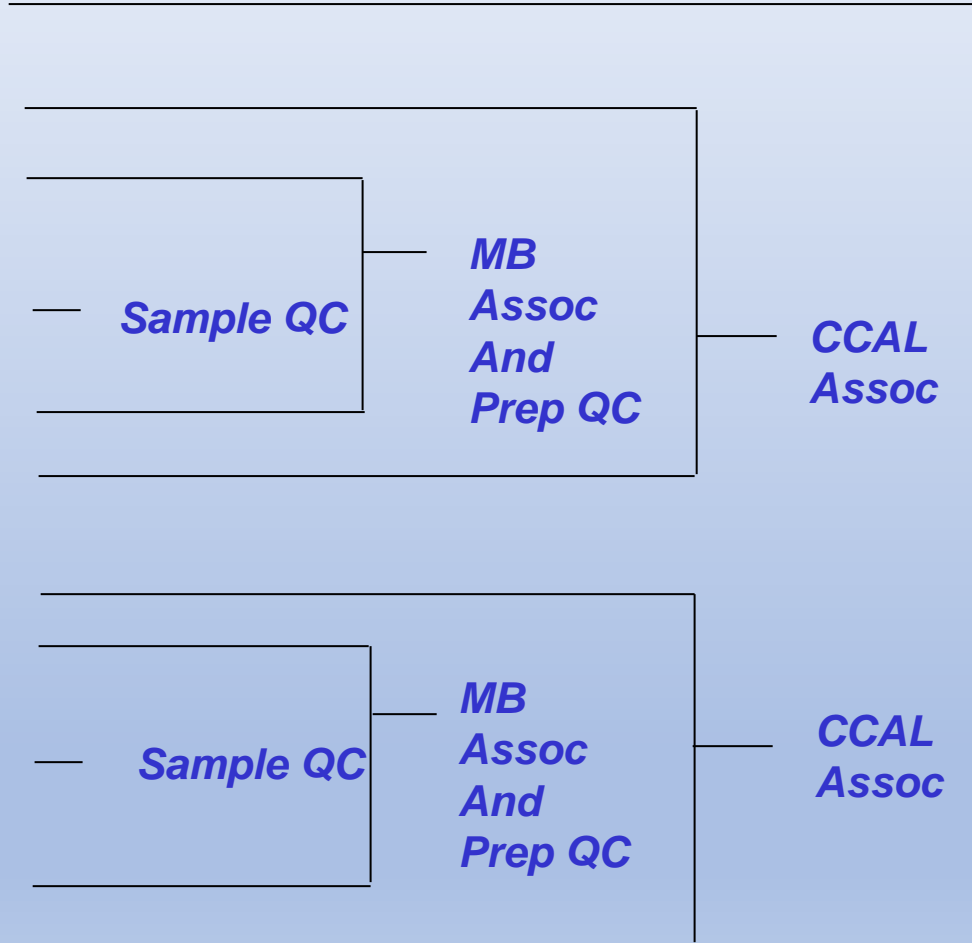
- Client Samples 1 - n

- Other QC
- Continuing Calibration Verification

- Tune
- Continuing Calibration Verification
- Method Blank/Negative Control
- Laboratory Control Sample
- Positive Control Sample

- Client Samples 1 - n

- Other QC
- Continuing Calibration Verification



ICAL Assoc

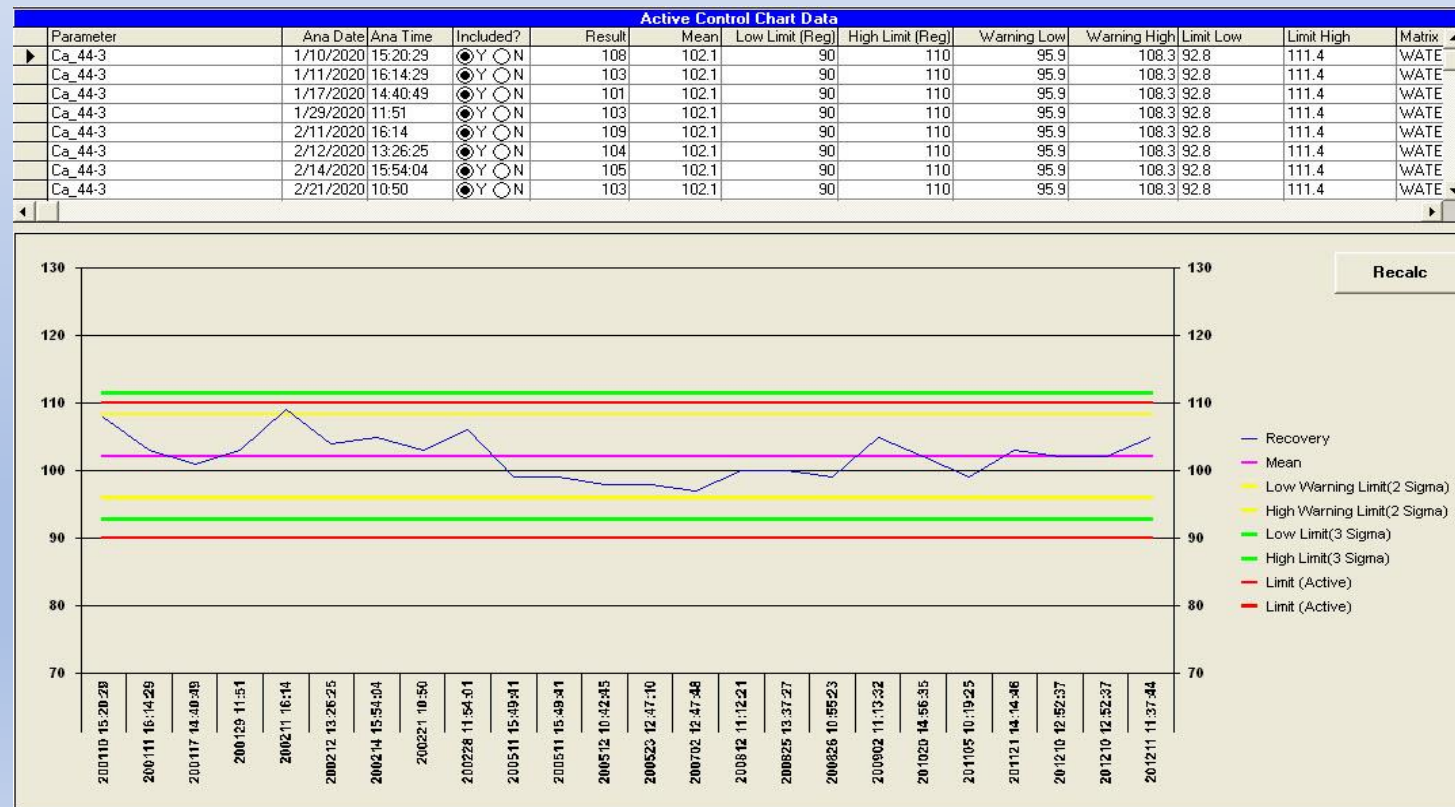
Key Batch Types

- Sampling Batch
- Shipping Batch
- Delivery Batch
- Storage Batch
- Raw Material Batch
- Manufacturing Batch
- Preparation Batch
- Analytical Batch
- Reporting Batch
- Compliance Batch

Pillars of Automated Data Integrity: Safety Assurance



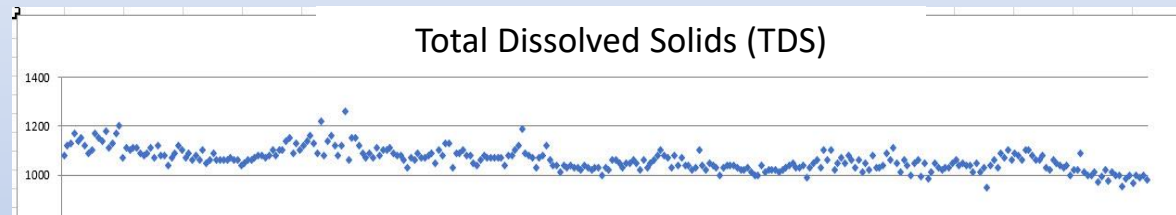
- QA Communication
 - Trending/Z-Scoring
 - Establish acceptance windows
 - Result comparisons



Trending – Z Scoring: Brings Anomalies to the Surface



Is something different occurring with the target sample?
Or did something go wrong during the process?



Parameter	Included?	Result	Mean	Z-Score	Sample ID	Z-Warning Low Limit	Z-Warning High	Z-Low Limit	Z-High Limit
Ca	Y	102	101.9667	0.007	C201090008	-2	2	-3	3
Ca	Y	103	101.9667	0.215	C201090009	-2	2	-3	3
Ca	Y	104	101.9667	0.423	C201090009	-2	2	-3	3
Ca	Y	108	101.9667	1.256	C2005010036	-2	2	-3	3
Ca	Y	110	101.9667	1.672	C2005010036	-2	2	-3	3
Ca	Y	110	101.9667	1.672	C2005010036	-2	2	-3	3
Ca	Y	107	101.9667	1.048	C2005010036	-2	2	-3	3
Ca	Y	100	101.9667	-0.409	C2007090031	-2	2	-3	3
Ca	Y	101	101.9667	0.201	C2007090031	-2	2	-3	3
Ca	Y	103	101.9667	0.215	C2007090031	-2	2	-3	3
Ca	Y	94.1	101.9667	-1.638	C2010060023	-2	2	-3	3
Ca	Y	96.2	101.9667	-1.2	C2010060023	-2	2	-3	3

Parameter	Ana Date	Ana Time	Included?	Result	Mean	Low Limit (Reg)	High Limit (Reg)	Warning Low	Warning High	Limit Low	Limit High	Matrix
Ca_44-3	1/10/2020	15:20:25	Y	108	102.1	90	110	95.9	106.3	92.8	111.4	WATE
Ca_44-3	1/11/2020	16:14:29	Y	103	102.1	90	110	95.9	106.3	92.8	111.4	WATE
Ca_44-3	1/17/2020	14:40:49	Y	101	102.1	90	110	95.9	106.3	92.8	111.4	WATE
Ca_44-3	1/29/2020	11:51	Y	103	102.1	90	110	95.9	106.3	92.8	111.4	WATE
Ca_44-3	2/11/2020	16:14	Y	109	102.1	90	110	95.9	106.3	92.8	111.4	WATE
Ca_44-3	2/12/2020	13:26:25	Y	104	102.1	90	110	95.9	106.3	92.8	111.4	WATE
Ca_44-3	2/14/2020	15:54:04	Y	105	102.1	90	110	95.9	106.3	92.8	111.4	WATE
Ca_44-3	2/21/2020	10:50	Y	103	102.1	90	110	95.9	106.3	92.8	111.4	WATE



Real-Time Z-Scoring Parameter Fluctuations

Real-Time QC Control Charts

Key Notification Alerts: Field Samples Outside Compliance Limits and QC Exceeding Acceptance Limits



- QC early detection builds a strong QA and risk aversion program for the lab
- Target result early detection builds a strong risk aversion program for the use of the results
- Early Detection – Rapid Response
- Proactive rather than reactive
- Experts can address issues early to minimize the severity of the problems

Pillars of Automated Data Integrity: Defensibility



- Communicating that all QA/QC was analyzed to ensure precision & accuracy of target results
- Monitor for instability or deviation in:
 - Method
 - Instrument
 - Preparation
 - Sampling
 - Preservation
 - Storage
 - Shipping

Key Elements of Defensibility



Primary Analytical Review Checklist

Documents

Reinitiate | Lists | Analyst Note(s) | View Checklist Item | Return

Analytical Review List

- All-Summary
- All-Checklist
- ICALs-% Relative Standard Devial
- ICVs-% Difference
- CCALs-% Difference
- Holding Times-Holding Time Extra
- Holding Times-Holding Time Analy
- MB Contamination-MB Contaminat
- ISTDs-Response Review
- ISTDs-Retention Time Review
- Surrogates-% Recovery
- Over Range-Over Range Review
- LCS/LCSD-% Recovery
- LCS/LCSD-% RPD
- MS/MSD-% Recovery
- MS/MSD-% RPD
- Associated Issues-Associated Par
- Detected Values-Detected Values
- Professional Judgements-Manual I

Checklist

Section	Seq	Checklist Item	Check Status	Report	Review Procedure	Analyst Notes
A	1	Summary of Analytical Sequence Issues	<input type="radio"/> Y <input type="radio"/> N <input checked="" type="radio"/> NA	flagdata2.rpt	Summary	
A	2	Business Analytical Review Checklist Report	<input type="radio"/> Y <input type="radio"/> N <input checked="" type="radio"/> NA	analytical-checklist.rpt	Checklist	

Sample Information

Sample ID	Client ID	Report?	QC Type	Ana Date	Time	Samp Wt/Vol	Extract Vol (uL)	Dil	% Moisture	Matrix	Z Flag	Data File	Rpt Units	Rt
CCAL-080102-1	ISC-50	<input checked="" type="checkbox"/>	CCAL/ISC	1/2/2018	11:08:21	10	10	1	100	WATER	N	L8010203.LC	ng/L	ST
VAP-23 (16-20)	VAP-23 (16-20)	<input checked="" type="checkbox"/>	SAM	1/2/2018	11:29:56	1000	1000	1	100	WATER	N	L8010204.LC	ng/L	ST
VAP-23 (26-30)	VAP-23 (26-30)	<input checked="" type="checkbox"/>	SAM	1/2/2018	11:51:43	1000	1000	1	100	WATER	N	L8010205.LC	ng/L	ST
VAP-23 (36-40)	VAP-23 (36-40)	<input checked="" type="checkbox"/>	SAM	1/2/2018	12:13:29	1000	1000	1	100	WATER	N	L8010206.LC	ng/L	ST
VAP-24 (26-30) MS	VAP-24 (26-30) MS	<input checked="" type="checkbox"/>	MS	1/2/2018	12:35:14	125	10	1	100	WATER	N	L8010207.LC	ng/L	ST
VAP-24 (26-30) MSD	VAP-24 (26-30) MSD	<input checked="" type="checkbox"/>	MSD	1/2/2018	13:09:18	125	10	1	100	WATER	N	L8010208.LC	ng/L	ST
VAP-23 (6-10) MS	VAP-23 (6-10) MS	<input checked="" type="checkbox"/>	MS	1/2/2018	13:30:53	125	10	1	100	WATER	N	L8010209.LC	ng/L	ST
VAP-23 (6-10) MSD	VAP-23 (6-10) MSD	<input checked="" type="checkbox"/>	MSD	1/2/2018	13:52:37	125	10	1	100	WATER	N	L8010210.LC	ng/L	ST
PBLK 17	PBLK	<input checked="" type="checkbox"/>	MB	1/2/2018	14:14:23	125	10	1	100	WATER	N	L8010211.LC	ng/L	ST
PLCS 17	PLCS	<input checked="" type="checkbox"/>	LCS	1/2/2018	14:51:44	125	10	1	100	WATER	N	L8010212.LC	ng/L	ST

Result Information

Parameter	CAS Number	Parm Type	Result Status	Report?	Detected?	Rpt Result	Rpt Rec	Rpt RPD	Rpt LOD	Rpt MDL	Rpt PQL	Rpt Truevalue	CQu
M3PFBS-IS		ISTD		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	800							
PFBS	375-73-5	MS/LCS TRC		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	286	114		1.42	0.74	1.42	250	
PFHpA	375-85-9	MS/LCS TRC		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	244	98		8.00	1.35	8.00	250	
M4PFHpA-IS		ISTD		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	800							
Br-PFHxS		MS/LCS TRC	Rerun due to LCS Low	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	25.8	10		3.44	1.60	4.00	250	
PFOA	335-67-1	MS/LCS TRC		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	256	102		2.00	0.376	3.20	250	
M8PFOA-IS		ISTD		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	800							
M2PFOA-S		SURR		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	37.39272	15					250	
T-PFOA		MS/LCS TRC		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	258	103		0	1.60	4.00	250	
M3PFHxS-IS		ISTD		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	800							
PFHxS		MS/LCS TRC	Rerun due to ISC Low-01/02/18-11:08:21	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	216	86		1.74	1.31	1.74	250	
M9PFNA-IS		ISTD		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	800							
PFNA	375-95-1	MS/LCS TRC		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	249	100		3.20	0.76	3.20	250	
Total PFHxS	355-46-4	MS/LCS TRC		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	242	97		3.44	0.83	4.00	250	
T-PFOS		MS/LCS TRC	Rerun due to LCS Low	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	40.5	16		4.00	1.60	4.00	250	
MPFOS-S		SURR		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	42.49128	17					250	
M8PFOS-IS		ISTD		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	800							
PFOS		MS/LCS TRC		<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	188	75		1.56	1.45	1.56	250	

Direct Qualification

Select/Deselect Samples

QC Association

Send to Reporting

Direct Qualification

Set Analysis Time

Defensibility - Analytical review of each sample type. Associated QC review with target samples.



- Must first align with:
 - Quality Assurance
 - Safety Assurance
- Method Performance, Precision, & Accuracy
- Analyst Competency
- Instrument Performance

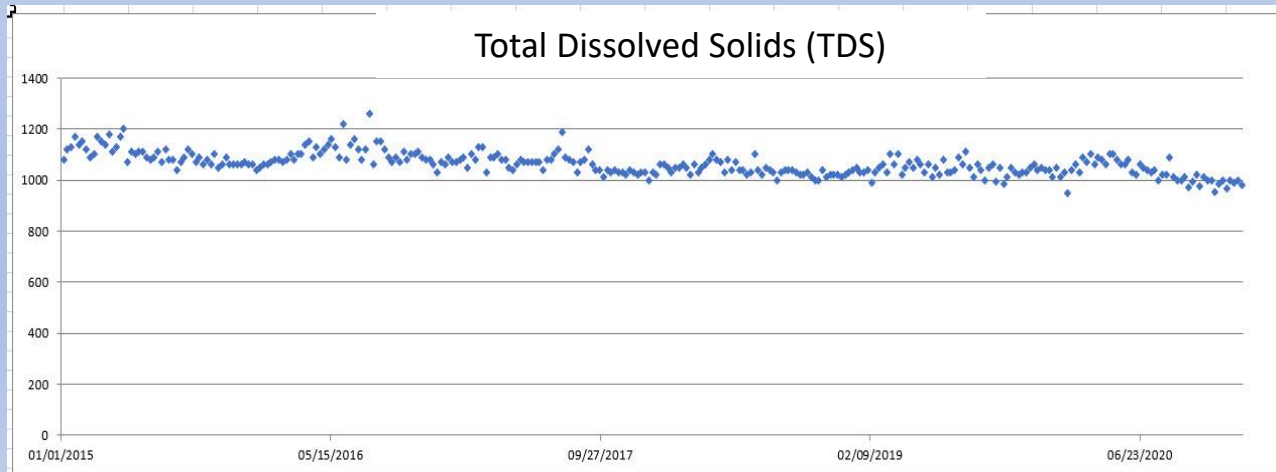
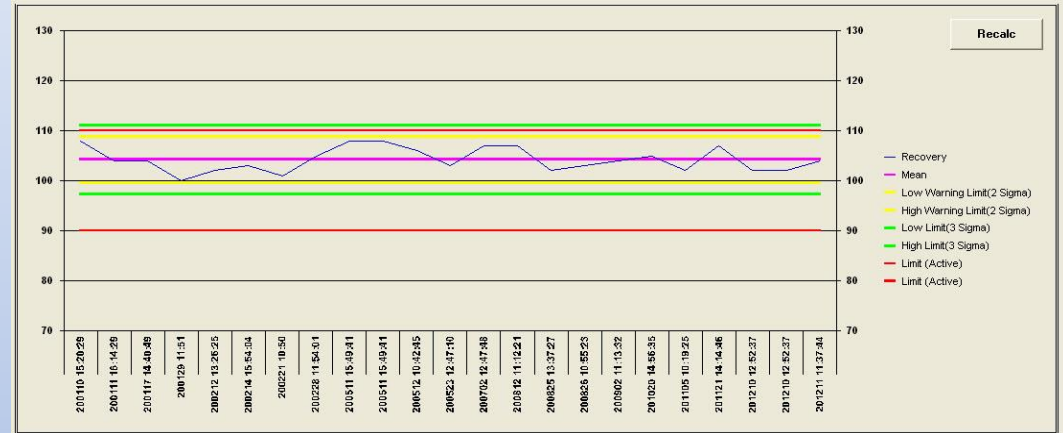
Key Elements of Reproducibility, Consistency, & Repeatability



Active Control Chart Data									
Parameter	Included?	Result	Mean	Z-Score	Sample ID	Z-Warning Low Limit	Z-Warning High	Z-Low Limit	Z-High Limit
Fe	Y	0.28	0.1075	1.755	C2001090008	-2	2	-3	3
Fe	Y	0.27	0.1075	1.653	C2001090008	-2	2	-3	3
Fe	Y	0.28	0.1075	1.755	C2001090008	-2	2	-3	3
Fe	Y	0.05	0.1075	-0.585	C2005010036	-2	2	-3	3
Fe	Y	0.06	0.1075	-0.483	C2005010036	-2	2	-3	3
Fe	Y	0.07	0.1075	-0.381	C2005010036	-2	2	-3	3
Fe	Y	0.06	0.1075	-0.483	C2007090031	-2	2	-3	3
Fe	Y	0.05	0.1075	-0.585	C2007090031	-2	2	-3	3
Fe	Y	0.06	0.1075	-0.483	C2007090031	-2	2	-3	3
Fe	Y	0.03	0.1075	-0.788	C2010060023	-2	2	-3	3
Fe	Y	0.04	0.1075	-0.687	C2010060023	-2	2	-3	3



Active Control Chart Data												
Parameter	Ana Date	Ana Time	Included?	Result	Mean	Low Limit (Reg)	High Limit (Reg)	Warning Low	Warning High	Limit Low	Limit High	Matrix
Fe_56-3	1/10/2020	15:20:29	Y	108	104.2	90	110	99.6	108.8	97.3	111.1	WATE
Fe_56-3	1/11/2020	16:14:29	Y	104	104.2	90	110	99.6	108.8	97.3	111.1	WATE
Fe_56-3	1/17/2020	14:40:49	Y	104	104.2	90	110	99.6	108.8	97.3	111.1	WATE
Fe_56-3	1/29/2020	11:51	Y	100	104.2	90	110	99.6	108.8	97.3	111.1	WATE
Fe_56-3	2/12/2020	13:26:25	Y	102	104.2	90	110	99.6	108.8	97.3	111.1	WATE
Fe_56-3	2/14/2020	15:54:04	Y	103	104.2	90	110	99.6	108.8	97.3	111.1	WATE
Fe_56-3	2/21/2020	10:50	Y	101	104.2	90	110	99.6	108.8	97.3	111.1	WATE
Fe_56-3	2/28/2020	11:54:01	Y	105	104.2	90	110	99.6	108.8	97.3	111.1	WATE





Ability to Trace Data Back to Its Source

- Prep analyst
- Instrument analysis
- Instrument software
- Processing software
- Analyst that performed the analysis
- Electronic signature
- Primary/secondary review
- Raw, meta & calculated results
- Audit trail

Key Elements of Traceability



Primary Analytical Review Checklist

Water Treatment Site

Reanalysis 1

Instrument

Acquisition

Analytical Notes

Failed CCV QC

Percent Solids

Analytical Dilution * Prep Factor

Analytical Batch

Prep Weights and Volumes

Analytical Method: M200_8ICPT

Section	Seq	Check Item	Check Status	Report
A	1	Printed Exception Report?	<input type="radio"/> Y <input type="radio"/> N <input checked="" type="radio"/> N	flagdata9v5
A	2	Internal Standards	<input type="radio"/> Y <input type="radio"/> N <input checked="" type="radio"/> N	flagdataintstd

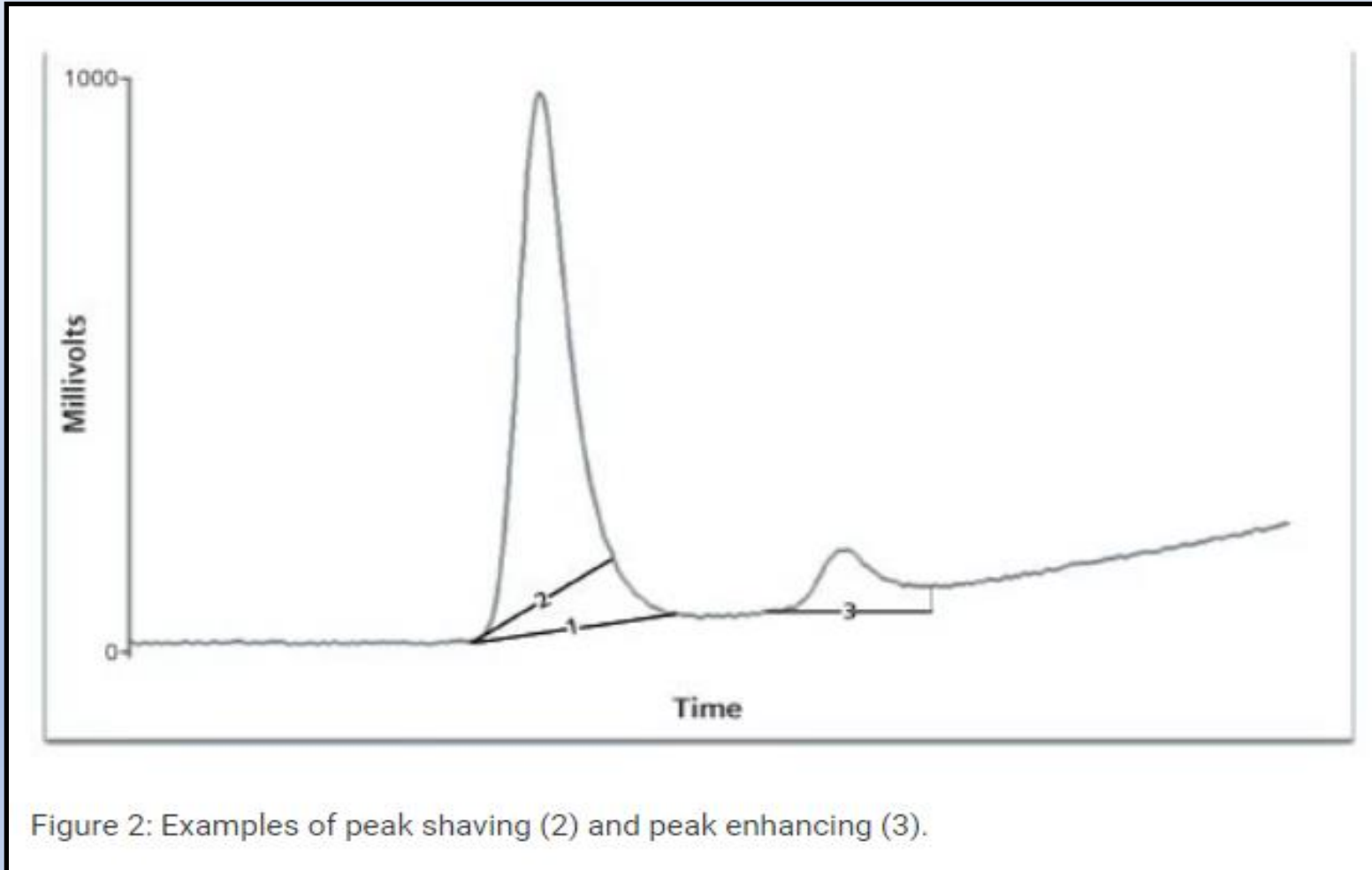
Pass/Fail	Lab ID	Sample ID	OR/URE	Rpt?	Inst ID	Ana Date	Time	QC Type	Dil	Batch Number	Found in LIMS?	Initial	Final	% Solids	Units	UM?	Tot/Diss
FAIL	420406	CCV1 for [METL/2178]		<input checked="" type="checkbox"/>	ICPMS2	6/1/2020	11:54	CCV1	1	2178	T	1	1	0	mg/Kg		Total
	420407	CCB for [METL/2178]		<input checked="" type="checkbox"/>	ICPMS2	6/1/2020	11:59	CCB	1	2178	T	1	1	0	mg/Kg		Total
	C2005120038	Shdgc	RE1	<input checked="" type="checkbox"/>	ICPMS2	6/1/2020	12:04	SAM	19.6	2178	T	0.2553	0.5	14.17	mg/Kg		Total
FAIL	420262	ShdgcMS	RE1	<input checked="" type="checkbox"/>	ICPMS2	6/1/2020	12:09	MS	19.9	2178	T	0.2517	0.5	14.17	mg/Kg		Total
FAIL	420263	ShdgcMSD	RE1	<input checked="" type="checkbox"/>	ICPMS2	6/1/2020	12:13	MSD	19.8	2178	T	0.2523	0.5	14.17	mg/Kg		Total
FAIL	420396	ShdgcPS	RE1	<input checked="" type="checkbox"/>	ICPMS2	6/1/2020	12:18	PS	19.6	2178	T	0.2553	0.5	14.17	mg/Kg		Total
	C2005270001	MAIN PLANT-Solids	RE1	<input checked="" type="checkbox"/>	ICPMS2	6/1/2020	12:23	SAM	20	2178	T	0.2506	0.5	26.62	mg/Kg		Total

Pass/Fail	Parameter	Storet Code	CC	Report?	Parm Type	Detected?	Rpt Result	Raw Result	Unit	UM?	Rpt Rec	Rpt TV	Rpt RPD	Response	Rpt PQL	Rpt DI
	Sr_88	01083	OK	<input checked="" type="checkbox"/>	REG	<input checked="" type="checkbox"/>	5.06	5.061	mg/kg	UM	101	5		5385808	0.50	0.07
	Y_89		OK	<input checked="" type="checkbox"/>	ISTD	<input type="checkbox"/>	1.400535E+07	1.400535E+07	CPS	UM	102.6	1.36507E+0		1.400535E+07		
	Y_89-2		OK	<input checked="" type="checkbox"/>	ISTD	<input type="checkbox"/>	1.200104E+07	1.200104E+07	CPS	UM	99.3	1.208213E+		1.200104E+07		
	Y_89-3		OK	<input checked="" type="checkbox"/>	ISTD	<input type="checkbox"/>	1894897	1894897	CPS	UM	97.2	1948815		1894897		
	Mo_95	01063	OK	<input checked="" type="checkbox"/>	REG	<input checked="" type="checkbox"/>	0.99	0.993	mg/kg	UM	99	1		208702.8	0.10	0.01
FAIL	Ag_107	01078	DR	<input type="checkbox"/>	REG	<input checked="" type="checkbox"/>	0.24	0.242	mg/kg	UM	48	0.5		140230.6	0.05	0.01
	Cd_111	01028	OK	<input checked="" type="checkbox"/>	REG	<input checked="" type="checkbox"/>	0.98	0.983	mg/kg	UM	98	1		122833.1	0.10	0.03
	In_115		OK	<input checked="" type="checkbox"/>	ISTD	<input type="checkbox"/>	1.356045E+07	1.356045E+07	CPS	UM	101.8	1.332213E+		1.356045E+07		
	Sn_118		NR	<input type="checkbox"/>	REG	<input type="checkbox"/>		0	mg/kg			250		347262.1		
	Sn_119	01103	OK	<input checked="" type="checkbox"/>	REG	<input checked="" type="checkbox"/>	0.96	0.957	mg/kg	UM	96	1		127072.8	0.10	0.04
	Sb_121	01098	OK	<input checked="" type="checkbox"/>	REG	<input checked="" type="checkbox"/>	0.97	0.97	mg/kg	UM	97	1		472006.5	0.10	0.01
	Ba_137	01008	OK	<input checked="" type="checkbox"/>	REG	<input checked="" type="checkbox"/>	0.94	0.943	mg/kg	UM	94	1		170485.4	0.10	0.02
	Tb_159		NR	<input type="checkbox"/>	ISTD	<input type="checkbox"/>		1.987681E+07	CPS			1.906574E-		1.987681E+07		
	Tb_159-2		OK	<input checked="" type="checkbox"/>	ISTD	<input type="checkbox"/>	1.742859E+07	1.742859E+07	CPS	UM	102.4	1.701832E+		1.742859E+07		
	Tl_205	01073	OK	<input checked="" type="checkbox"/>	REG	<input checked="" type="checkbox"/>	0.94	0.944	mg/kg	UM	94	1		883447.3	0.10	0.02
	Pb_206	01052	NR	<input type="checkbox"/>	ISTD	<input type="checkbox"/>		335479.1	mg/kg					335479.1		



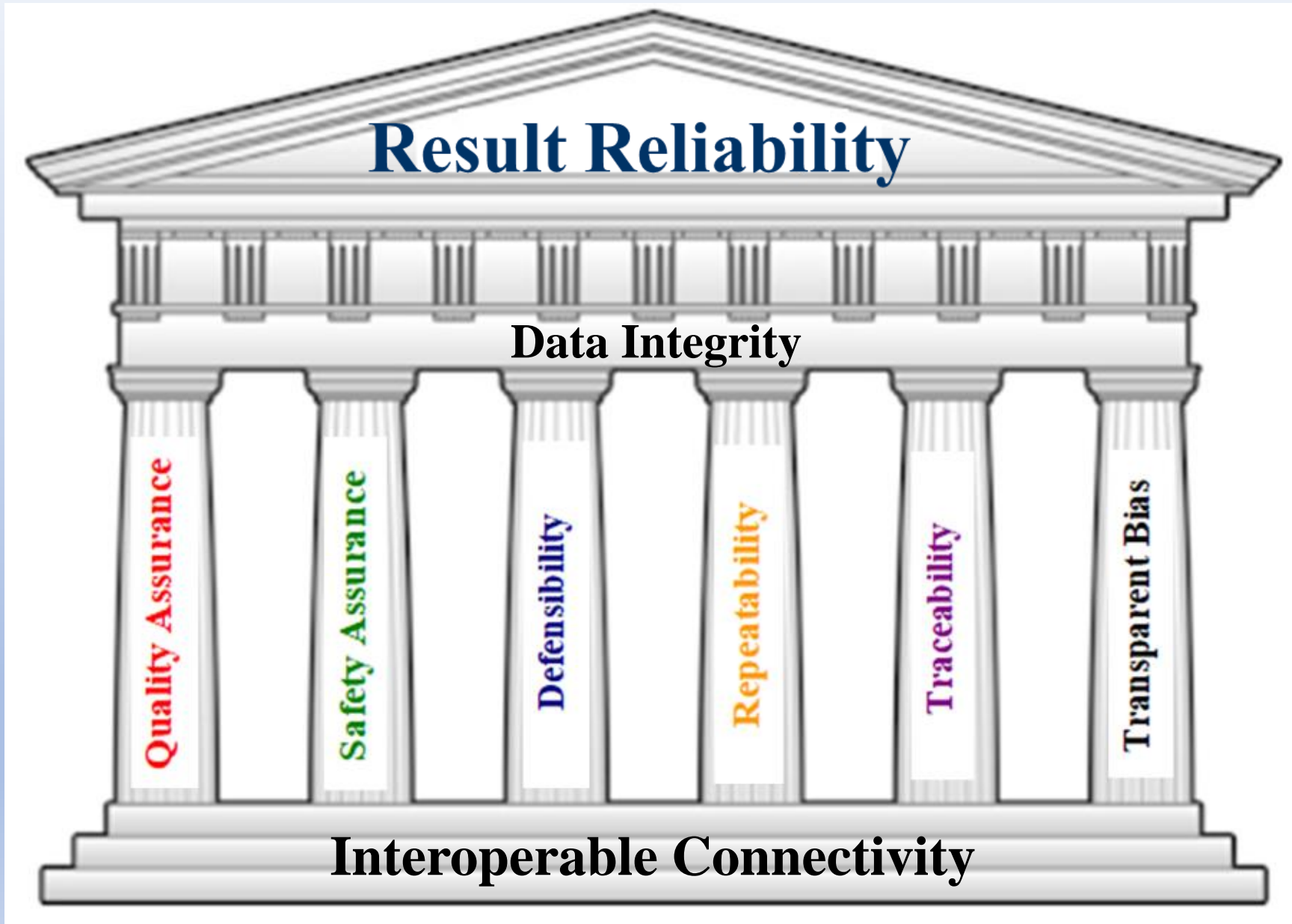
- Capture
 - Manual integrations
 - Deletion of interfering peaks
 - Professional judgments
 - Professional notes
 - Professional comments

Professional judgments that are hidden or unknown become biases for the use of the results.

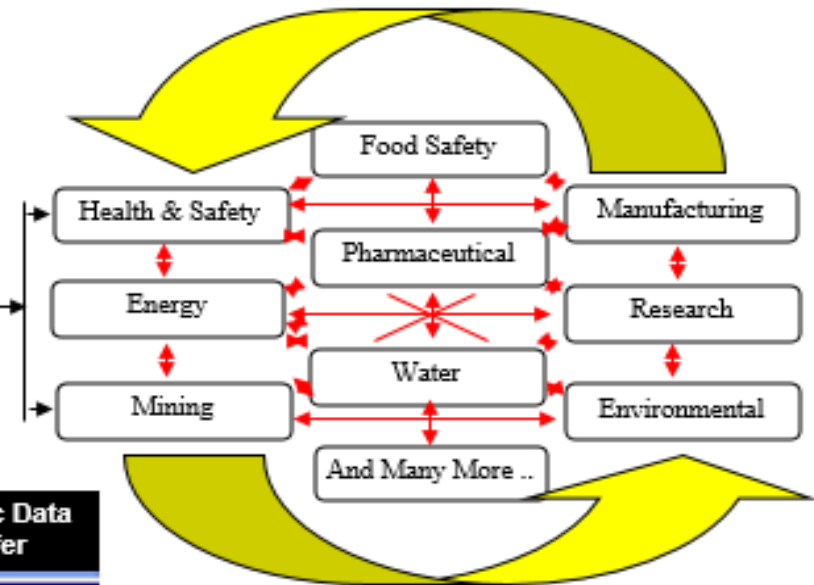


Continual monitoring for:

- **Bad Habits**
- **Poor Judgments**
- **Shortcuts**



Seamless Process Flow



EISC = Scientific Data Exchange



Entire process takes just minutes vs. hrs/days/mths
Saves time, money, and get the right answer.

Steps to Automated Data Integrity



One Instrument, One Analysis at a Time

- Choose a Key Instrument and Analysis
- Determine Notification Alerts
- Determine Quality Control
- Determine Deliverables Required
- Connect to the Lab's Additional Data Sources
- Creates Template for Next Instrument and Analysis

Thank you!

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