PFAS Litigation and Regulatory Developments Conference

LITIGATION MANAGEMENT AND THE USE OF AI

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False Positives, False Negatives, and Interferences:
A Deep Dive into the PFAS Data

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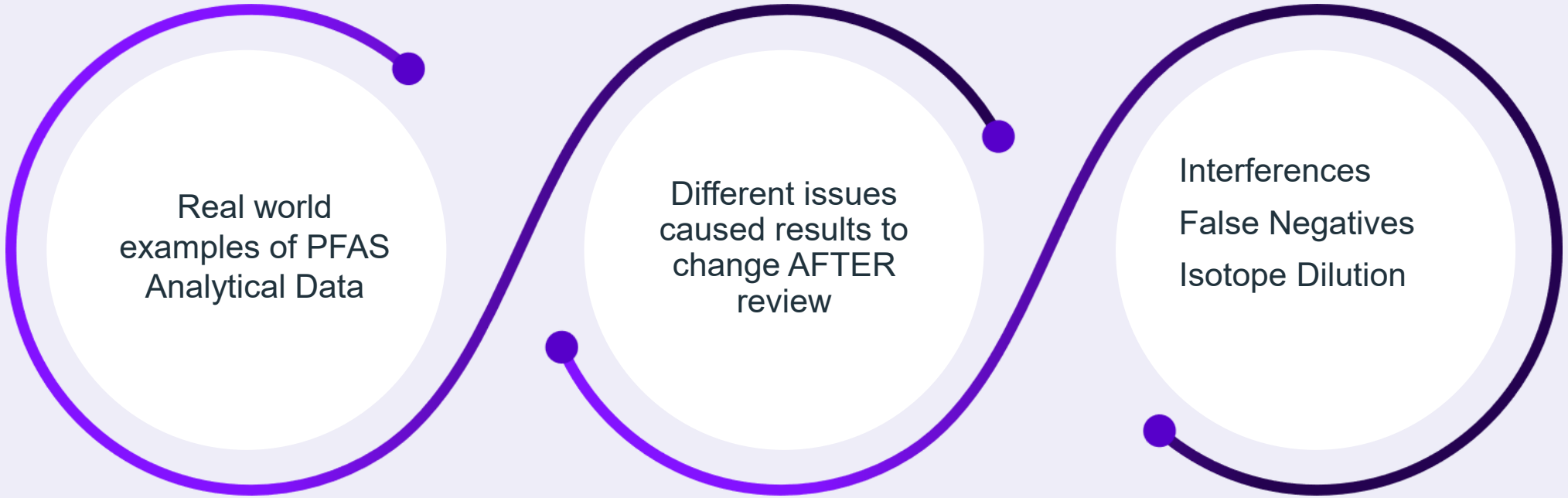
Why Do We Need to Evaluate the Lab's Data?

- Data may be used to make costly decisions
- Data may have potential to impact human health
- Need to confirm quality data available and appropriate to support decisions
- Need to determine potential low or high biases, potential uncertainties, potential false positive or false negative results

Even if the lab follows all method-required procedures, there can still be data quality/usability issues.

Today's Presentation



"Level 2" versus "Level 4" Data Packages

False Positives/ Interferences

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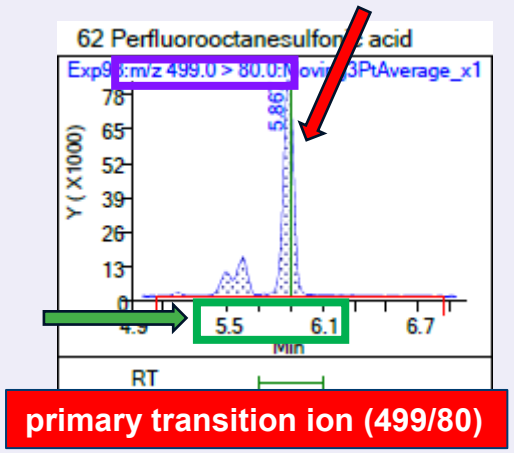
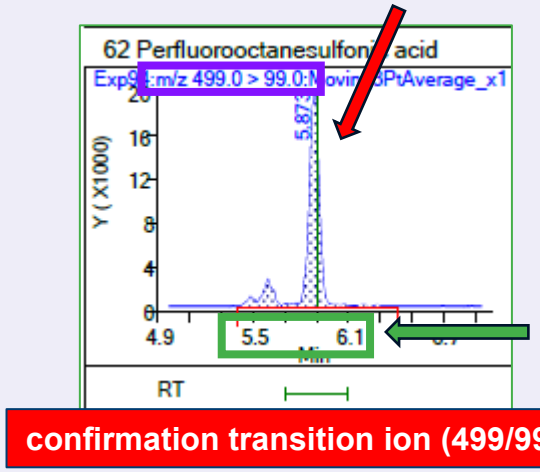
How is a PFAS Compound Positively Identified in the Laboratory?

PFOS Primary ion



primary transition ion (499/80)

PFOS Confirmation ion



confirmation transition ion (499/99)

1. **What is the retention time of the PFAS compound?** What time does it elute from the LC?
   - Look at chromatogram x-axis
   - Look at quantitation report: actual RT and expected RT reported
   - Ensure that RT is correct (close to expected RT)
2. **Are both the primary and confirmation transition ions present?**
   - Look at chromatogram
3. **Is the ratio of the primary ion to the confirmation ion within the acceptance criteria?**
   a. Look at quantitation report.
   b. 470063 / 95031 = 4.95
   c. Ion ratio acceptance criteria: 2.45-7.34

Analyte	Retention Time (min)
PFBS	4.79
PFOS	5.87
PFOA	7.22

Laboratory Quantitation Report

Signal	RT	EXP RT	DLT RT	REL RT	Response	Amount ng/ml	Ratio(Limits)
62 Perfluorooctanesulfonic acid							
499.0 > 80.0	5.867	5.885	-0.018	1.000	470063	1.78	Target=4.90
499.0 > 99.0	5.873	5.885	-0.012	1.001	95031		4.95(2.45-7.34)

Analyte	Ion Ratio	Ion Ratio Limit
PFBS	2.91	1.35-4.05
PFOS	4.95	2.45-7.34
PFOA	3.0	1.72-5.10

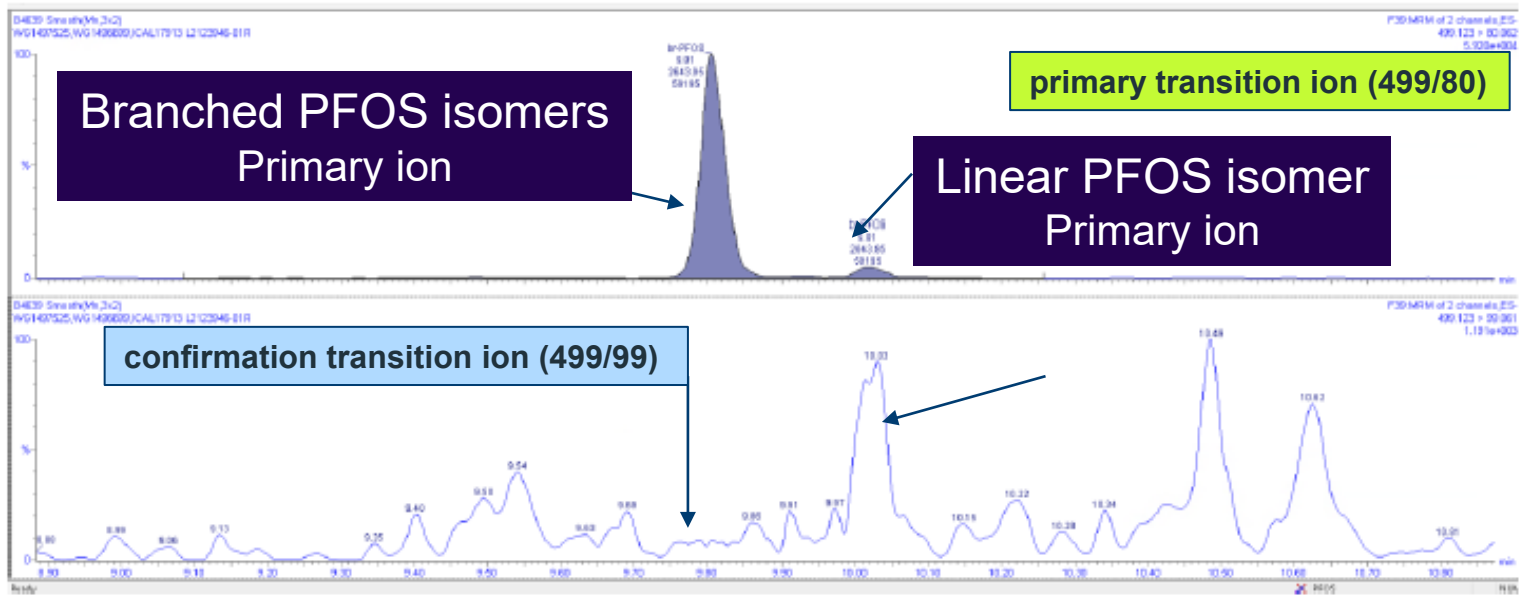
Confirmation Ions: Few More Things

- **If ion ratios are outside limits, what does this mean?**
  - Potential presence of interference
  - Potentially suspect positive result
- **What if there is no confirmation ion?**
  - PFBA
  - PFPeA
  - NMeFOSE
  - NEtFOSE
  - PFMPA
  - PFMBA

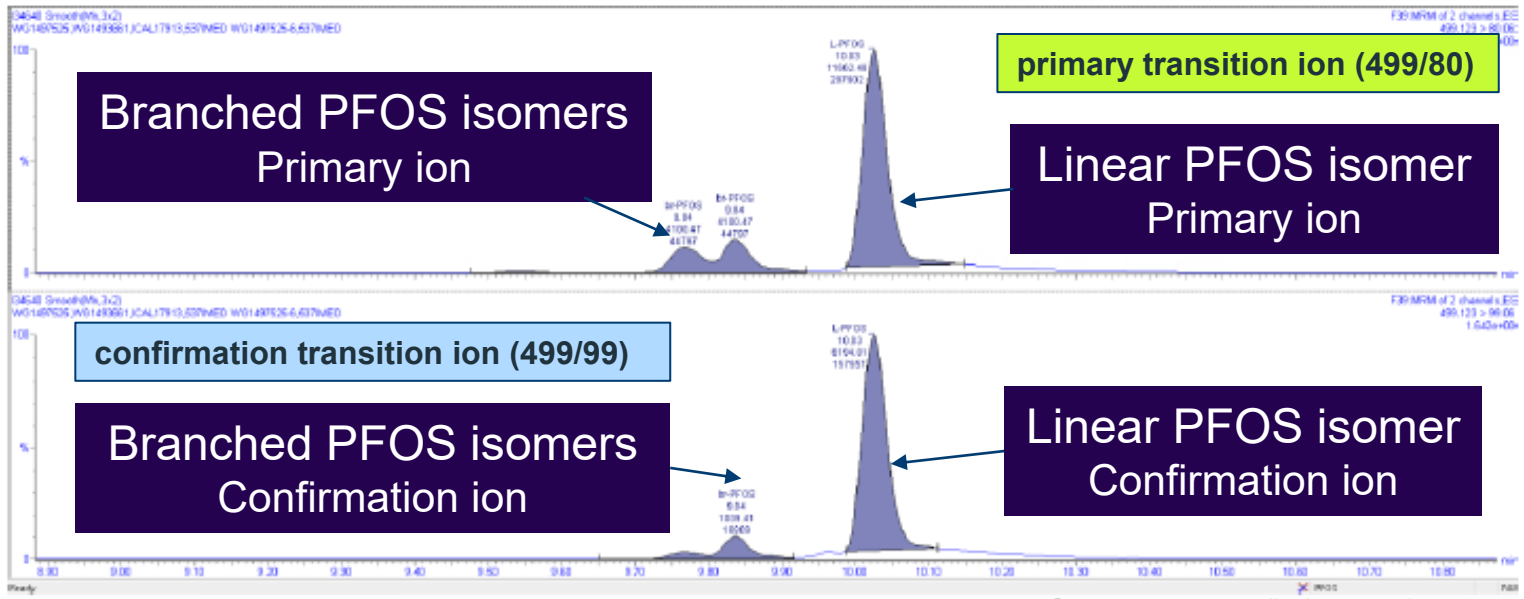
Examples			
Analyte	**Ion Ratio**	**Ion Ratio Limit**	
PFOS	2.91	2.04-6.12	Ok
PFOS	4.19	2.04-6.12	Ok
PFOS	8.20	2.04-6.12	Out

NOTE:
EPA Method 1633A and 537.1 require the use of confirmation ions.
EPA Method 533 does not require confirmation ions.

Sample



10 ng/ml CCV



Issue:

- Sample first analyzed using EPA Method 533
  PFOS = 2,680 ng/L
- Asked lab to reanalyze using Modified 537

Observations:

- PFOS peaks in sample did not produce ion ratio signatures similar to standard
- Not all branched isomers of PFOS produce same confirmation ion: can make identification of branched PFOS isomers questionable since not monitoring all confirmation ions

How Should Lab Report This?

- If 533, report as is.
- If 1633 or 537 mod, may vary by lab:
  - ND due to lack of confirmation ion
  - As is with knowledge that not all branched PFOS isomers produce same conf ion
  - As is with ion ratio qualifier (e.g., “I”, “F”)

Ion Ratios out: Detection or Nondetect?

Bile Acid Interferences

Compound	Parent Ion	Primary Ion	Confirmation Ion
PFOS	499	80	99
TDCA	498	80	107
TCDCA	498	80	107
TUDCA	498	80	107

- **PFOS reported as false positive in samples since Bile Acids have common transition ion (80)**
- **PFOS also measured using 499→99 allowing Interference to be eliminated**

Lessons Learned

- Ask the lab when something does not look right.
- Ion ratio anomalies and interference with PFOS can be common.
- Think about this issue for any historical PFOS data you are looking at.
- Remember EPA method 533 does not require the use of confirmation ions.

False Negatives

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Field Duplicate Results from Level 2 Report

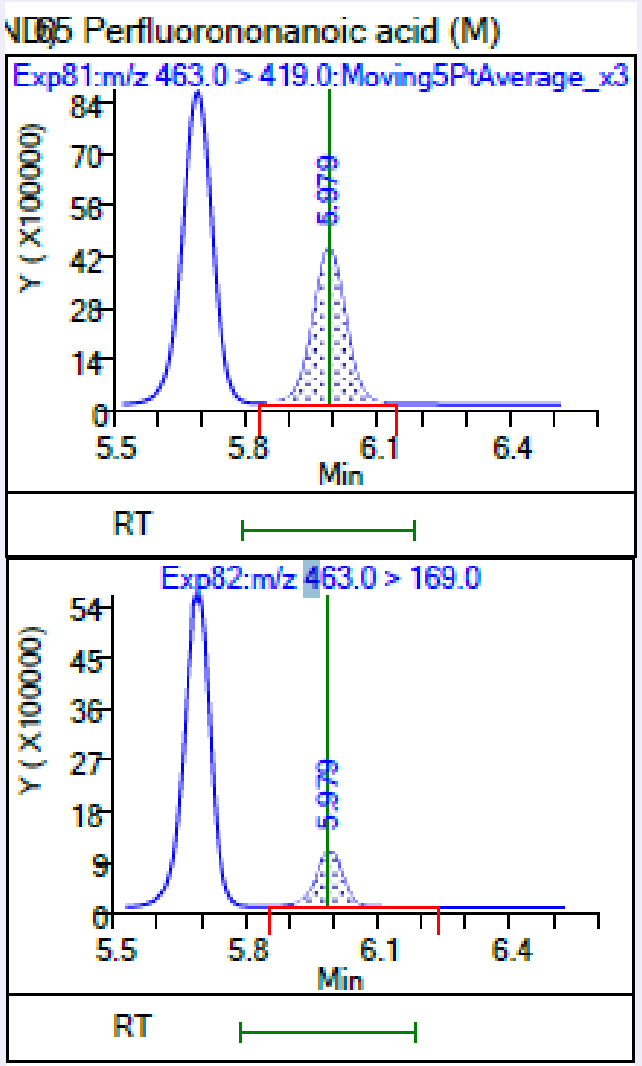
PFAS	GW Sample (ng/L)	Field Duplicate (ng/L)
PFOA	33	31
PFBS	1.4 J	1.3 J
PFHxS	0.96 J	0.82 J
PFOS	5.4	5.0
PFNA	290	1.8 U

Issues:

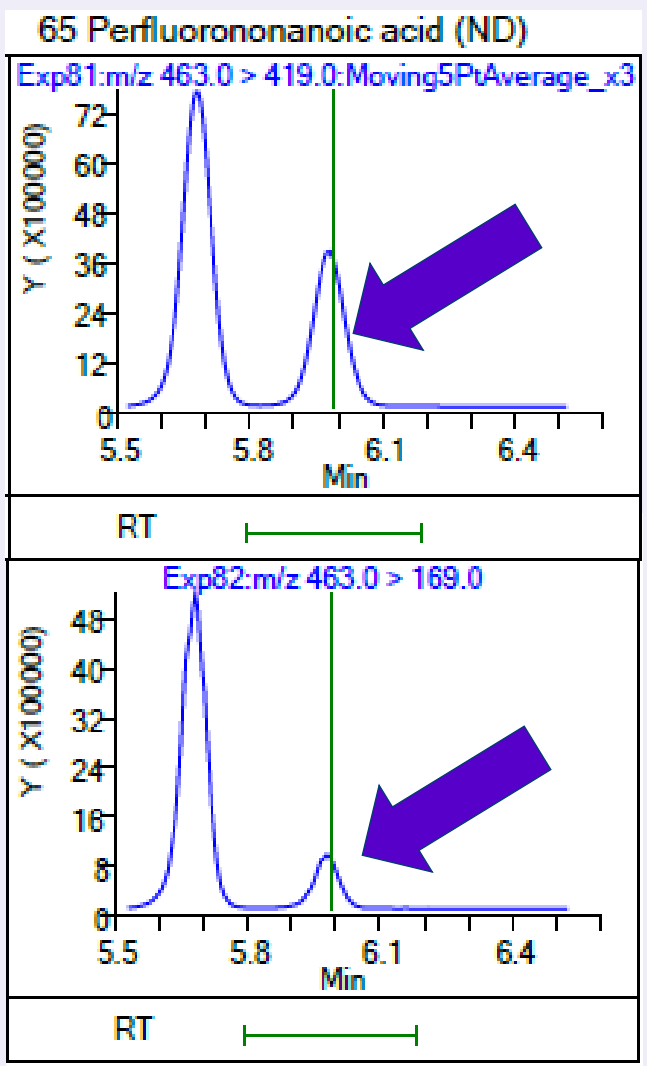
- Reviewing a Level 2 Report
- PFNA results did not look right

Missing Peak Integrations

GW Sample



Field Duplicate



- We happened to also have Level 4 reports.
- Upon review, noticed PFNA not integrated in field duplicate sample.
- Requested lab revise and review all other data generated for project.

PFNA (ng/L)	
Before	After
1.8 U	9.2
1.8 U	16
1.8 U	1.4 J
1.8 U	290
1.8 U	14
1.9 U	14
1.9 U	1700
1.9 U	350
1.9 U	620
1.9 U	350

Regulatory Criteria:
20 ng/L
(sum of 5 PFAS)

PFHpA (ng/L)	
Before	After
1.7 U	12
1.9 U	22
1.7 U	11
1.7 U	7.5
1.8 U	14
1.8 U	1.6 J
2.0 U	23
1.7 U	5.9
1.8 U	9.0
1.8 U	6.7

Regulatory Criteria:
20 ng/L
(sum of 5 PFAS)

After Lab Reviewed all Peaks for Missing Integration

- Revised data showed false negative results originally reported
- Some of revised data went from ND to causing a regulatory criteria exceedance

Why Did This Happen?

- All errors were due to one analyst who was not properly trained
- Proper secondary review had not been performed in the lab to catch this error prior to reporting

Isotope Dilution
(but not really)

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Isotope Dilution

- **True isotope dilution:** response of target analyte is compared to response of its isotopically labeled analog (EIS). 24 target PFAS quantified in this way in EPA 1633.
  - 13C4-PFBA used to quantify PFBA
  - 13C8-PFOA used to quantify PFOA
  - 13C8-PFOS used to quantify PFOS

- **Extracted internal standard quantification:** response of target analyte is compared to response of isotopically labeled analog of another compound with chemical and retention time similarities. 16 target PFAS quantified in this way in EPA 1633.
  - 13C3-PFHxS used to quantify PFPeS (5-carbon sulfonic acid)
  - 13C8-PFOS used to quantify PFNS (9-carbon sulfonic acid)
  - 13C5-PFPeA used

$$\text{Concentration Target} = \frac{\text{Target Area} * \text{True Concentration Isotope}}{\text{Area EIS} * \text{Calibration Factor}}$$

Table 10 in EPA 1633 (... get PFAS

How Did The Lab Quantify PFAS?

Remember: EIS used to quantify PFAS should have chemical and retention time similarities to target PFAS (it is supposed to mimic behavior of target PFAS)

PFHpS	5:3 FTCA	PFNS, PFDoS	PFTrDA	9Cl-PF3ONS
Quantified with: 13C6-PFDA	Quantified with: 13C8-PFOS	Quantified with: 13C7-PFUnA	Quantified with: D7-MeFOSE	Quantified with: 13C4-PFHpA
7-carbon sulfonic acid quantified using 10-carbon carboxylic acid	carboxylic acid quantified using sulfonic acid	9 and 10-carbon sulfonic acid quantified using 11-carbon carboxylic acid	carboxylic acid quantified using sulfonamido ethanol	ether sulfonate quantified using carboxylic acid

How Did This Impact Results?

Target PFAS	PFPeS	PFHpS	PFNS	PFDoS	PFDS	9Cl-PF3ONS	11Cl-PF3OUdS	3:3 FTCA	PFMPA	5:3 FTCA	7:3 FTCA
EIS Used by Lab	13C3-PFBS	13C6-PFDA	13C7-PFUnA	13C7-PFUnA	D5-EtFOSA	13C4-PFHpA	13C5-PFPeA	13C4-PFBA	13C4-PFBA	13C8-PFOS	13C8-PFOSA
EIS Required to be Used by Method	13C3-PFHxS	13C8-PFOS	13C8-PFOS	13C8-PFOS	13C8-PFOS	13C3-HFPO-DA	13C3-HFPO-DA	13C5-PFPeA	13C5-PFPeA	13C5-PFHxA	13C5-PFHxA
Sample 1											
%R of EIS Required to Be Used by Method	77%	51%	51%	51%	51%	55%	55%	10% *	10% *	43%	43%
%R of EIS Used by Lab	30%	49%	32%	32%	23%	63%	10% *	2% *	2% *	51%	63%
	Result biased high	No sig. effect	Result biased high	Result biased high	Result biased high	Result biased low	Result biased high	Result biased high	Result biased high	Result biased low	Result biased low

Takeaways

If the data do not make sense to you, ASK THE LAB!

In general, labs are doing a good job with PFAS analysis but errors or poor judgment can happen.

Reviewing raw data (Level 4 reports) can be more costly but can also give you more assurance in accuracy of your data.

Recommended Strategies: Guardrails

- The real danger is false confidence

- Proceed with caution
  - AI Hallucinations haunting the legal industry
  - Hallucinated data could cost you and your client
    - Ex) 1B GPY vs. 100M GPY

- Do not delegate negotiation, settlement judgment, or legal strategy to AI

- AI can accelerate work, but the lawyer still owns the filing, the facts, and the strategy

Recommended Strategies: Start small, closed, and defensible

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- Good first AI tasks: unit conversions (e.g., GPM to GPY conversions), data cleanup, chronologies, transcript summaries
- Use only closed-environment AI tools to avoid disseminating confidential or privileged materials
- Treat AI like a fast junior associate (useful for first drafts, but not final judgment)
- Require a mandatory human QA step before anything is filed, served, or used to support a claim

High Volume of Cases: Use AI to create structure, not autopilot

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- AI is best at triage → organize various documents, compare and contrast data, flag inconsistencies
  - Ex) Upload dozens of publicly available pleadings and prompt AI to compare and contrast
- Public water systems and municipalities → reconcile flow rate data and testing history (especially for PWS with dozens of water sources)
  - Potential non-legal use of AI → blend water sources (utilizing lower PFAS water sources)
- Personal injury cases → utilize UCMR 5 data in conjunction with clients' PWS IDs; identify qualifying diagnosis and build medical chronologies
  - Future AI use → simultaneous AI cross-matter review
    - Ex) AI tools to scan documents (medical records, work histories, housing records) to populate data in your CRM and plaintiff fact sheets

Thanks!

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