

Emerging Technologies and Increasing Data Interpretation Concerns

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Interpretation and Use of Analytical Data: Potential Concerns

- **Forensic Investigations Requiring Trace Analyses for Unique Analyte Classes**
 - **Use of MDL reporting for lowest levels of reporting**
 - **Use of newer technologies for more sensitive analyses**
- **Increased Risk of False Positive Results with Use of MDL Reporting**
 - **Lack of Verification of precision and accuracy through use of verification standards**

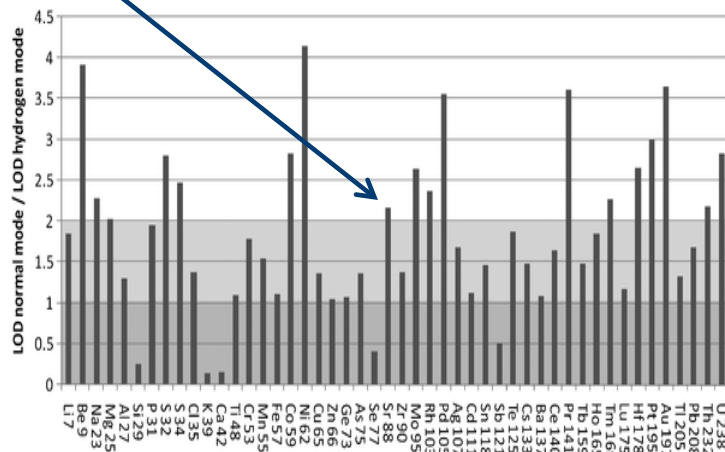
A Few Definitions

- **LOD** - the lowest amount of analyte in a sample that can be detected, but not necessarily quantitated as an exact value.
- **MDL** - The method detection limit is defined as the minimum concentration of a substance that can be measured and reported with 99% confidence that the analyte concentration is greater than zero and is determined from analysis of a sample in a given matrix containing the analyte.
- **LOQ** - the lowest amount of analyte in a sample that can be quantitatively determined with acceptable precision and accuracy

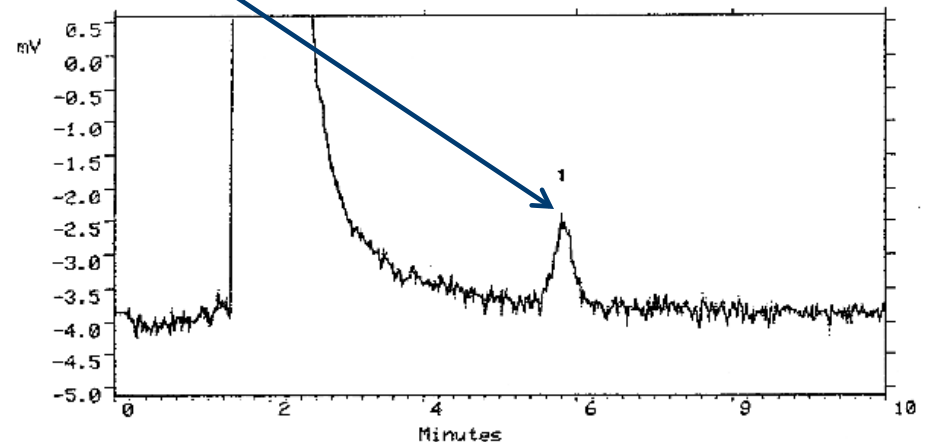
Limit of Detection

- There are two kinds of detecting...
 - As in ICP... you don't detect this analyte until you are out of the background range; or as in GCMS, where the analyte starts to appear with distinguishable characteristics

ICP



GCMS



Limit of Detection

- **Analyses that have high specificity for analyte identification, using multiple sources of identification criteria (retention time, ions, ion ratios, chemistry, prep) – LIKE GCMS – don't have the same false positive problems as inorganic ICP and ICPMS analyses...**
- **We can estimate the potential for false positive results when using the MDL by evaluating the frequency of positive results above the MDL in method blank data**

Analyte	40 CFR Determined MDL	Average Blank Concentration	Standard Deviation of Blank Concentration
Aluminum	10.23	4.7	5.23
Antimony	0.0168	0.109	0.0886
Arsenic	0.0168	0.0292	0.0971
Beryllium	0.0613	0.0105	0.0339
Cadmium	0.0153	0.00591	0.023
Chromium	0.25	0.138	0.276
Cobalt	0.1057	0.0065	0.0254
Copper	0.2497	0.102	0.196
Lead	0.0819	0.0141	0.0238
Manganese	0.1109	0.185	0.442
Molybdenum	0.047	0.373	0.513
Nickel	0.0819	0.0157	0.034
Selenium	0.0382	0.0045	0.0274
Silver	0.1023	0.0141	0.0313
Thallium	0.0153	0.00714	0.0318
Vanadium	0.13	0.311	0.193
Zinc	0.61	1.26	2.01

Larger Data Population

Let's Review Data from 19 Labs

- Actual reported results from samples based on requirement to report to the MDL as defined by 40 CFR Part 136: 138,212 reported results
- 5,043 reported results between MDL and RL in samples, or 3.6%
- Expected number based on detections in blanks is 3,511, or 2.3%
- If the frequency of false positives in samples is the same as that in blanks, 3511 of these results would be false positives
- So, of those results below between MDL and RL, 70% *might* be false positives

Conclusion

- For most analytes we can be confident that we are not reporting false positives when reporting to the MDL because we essentially never see them in blanks.
- For a subset of the analytes, including many that are environmentally significant, the risk of false positives when reporting to the method detection limit is significant.
- For positive results reported between the MDL and the RL, our best estimate of the potential false positive rate is approximately 25%.
- Batch method blanks, taken in isolation, will not reliably indicate whether a positive result in a sample less than the RL is a false positive.