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

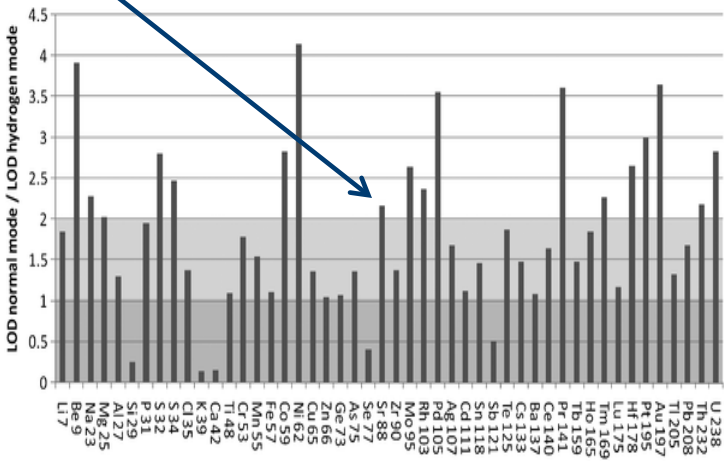
A Few Definitions

- **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**

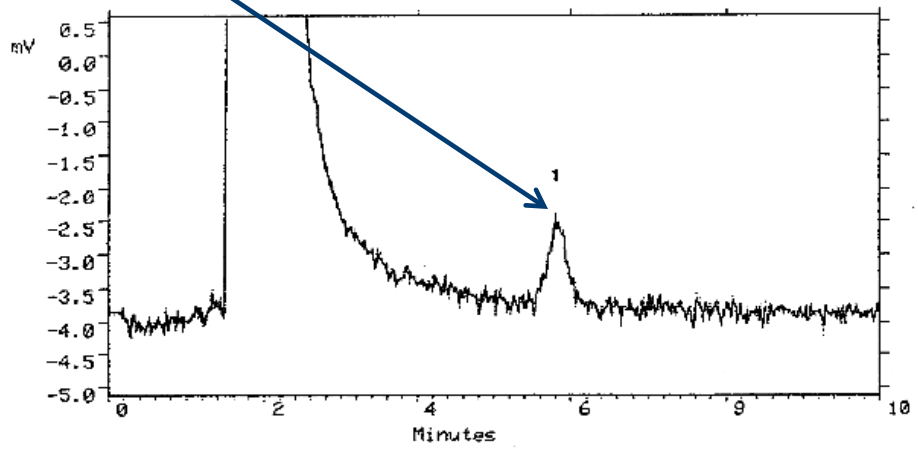
Limit of Detection

- **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.**