

TestAmerica

THE LEADER IN ENVIRONMENTAL TESTING

**45th Annual
Environmental Show of the South**

Conference & Exhibition

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Gatlinburg, Tennessee

**The Fundamentals of
Organic Compound Quantification
(Part I)**

**Presented by: William C. Anderson, Ph.D.
TestAmerica Laboratories, Inc.
Knoxville, Tennessee**

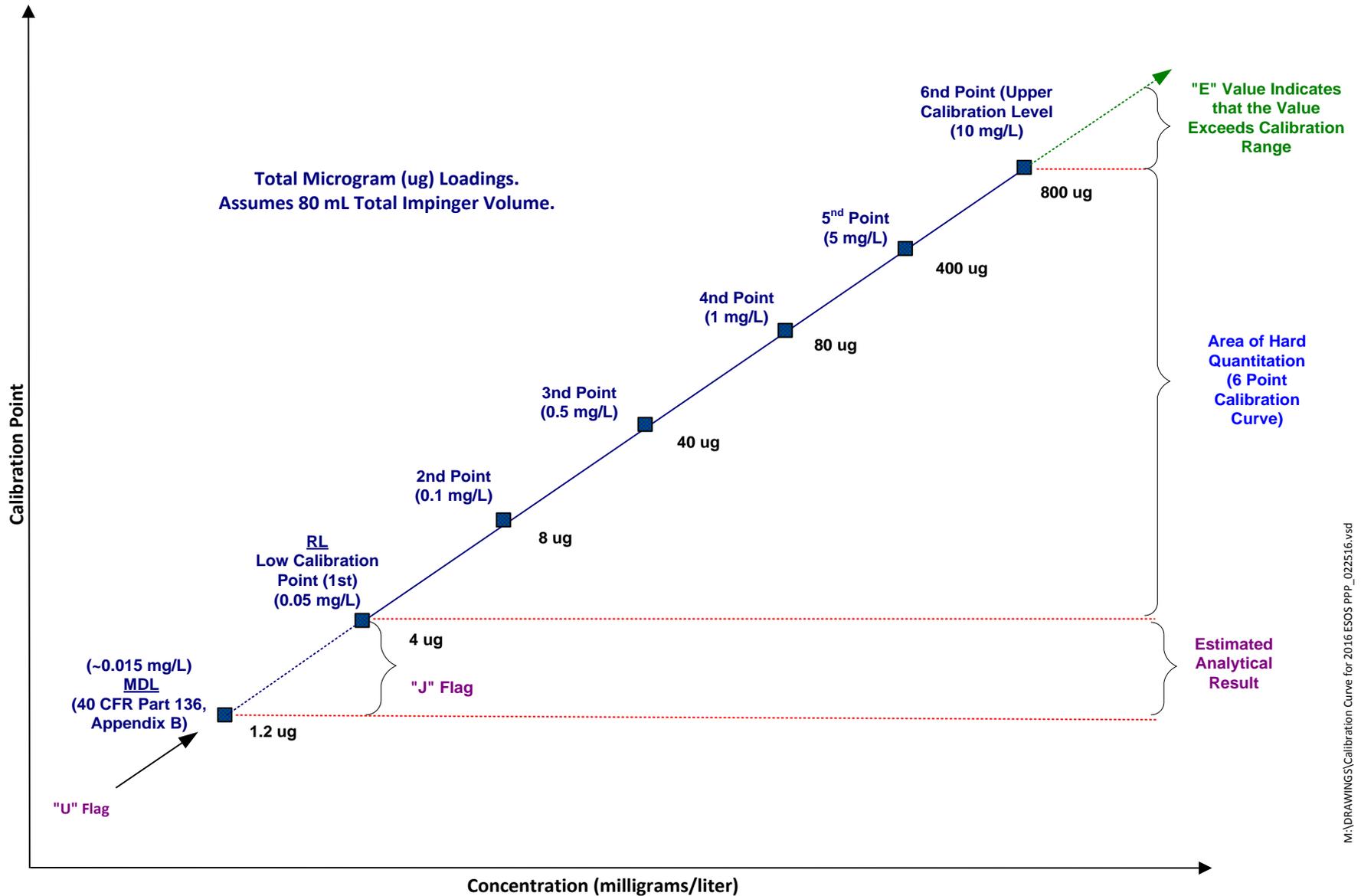
Quantification of Organic Compounds

✓ **Calibrations and Data Flags**

✓ **The Use of Surrogates**

✓ **The Use of Internal Standards**

Example Calibration Curve Showing the Regions of Estimated Analytical Results and Hard Quantitation Results During Analysis



Detection Limit versus Quantification Limit

What is the Reporting Limit or RL?

- ✓ **Defines where quantification is commenced without data flags**
- ✓ **Defines “hard quantification”**
- ✓ **Data is bracketed by calibration points**

What is a Method Detection Limit or MDL?

- ✓ Is statistically determined
- ✓ Is level that says with 99% confidence that a “hit” is greater than zero
- ✓ Since the MDL is statistically derived, it has a confidence interval around it

The Implications are Important!

Example: If MDL = 2 ppb

**At a 95% confidence interval,
what is the range from the upper
and lower confidence levels?**

At 2 ppb:

1.28 ppb → 2 ppb → 4.4 ppb

At a concentration of the analyte at 2 ppb, we are 99% confident that the analyte will be detected. Our ability to find 2 ppb with 95% confidence limits is represented by a range of results from 1.28 to 4.4 ppb.

Statistically they are the same number!

The MDL was Promulgated in 1984.

40 CFR Part 136, Appendix B.

See “Development of Compliance Levels from Analytical Detection and Quantitation Levels”

EPA Document Number PB95-216321

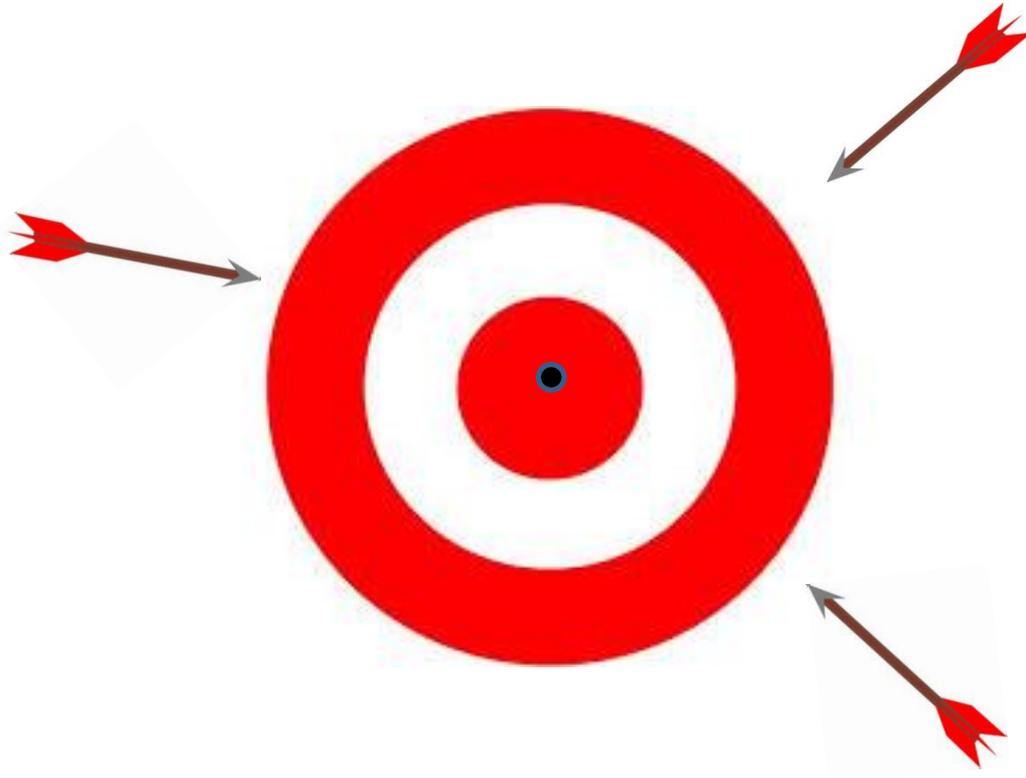
Precision and Accuracy

Precise, But Not Accurate



Precision and Accuracy

Accurate, But Not Precise



Precision and Accuracy

Accurate and Precise



The Use of Surrogates

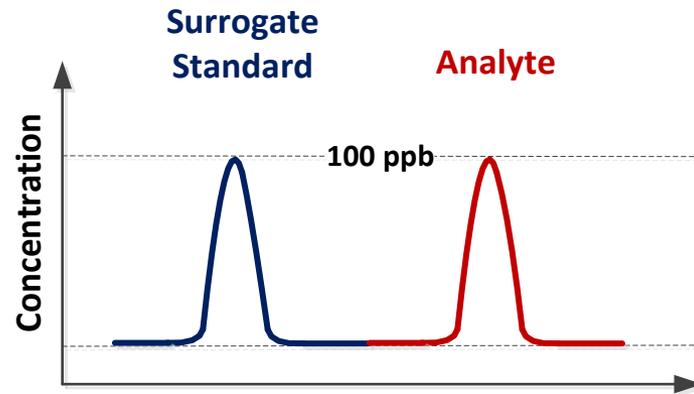
Definition and Description of Use

Examples of Chemistry at Work

A surrogate is a chemically similar compound to the ones being investigated but not expected to occur in the environmental samples.

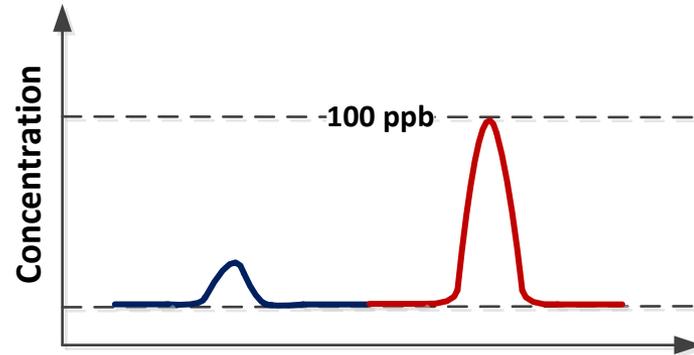
The final data is not adjusted for surrogate recoveries.

Surrogate Standard Spiked @ 100 ppb



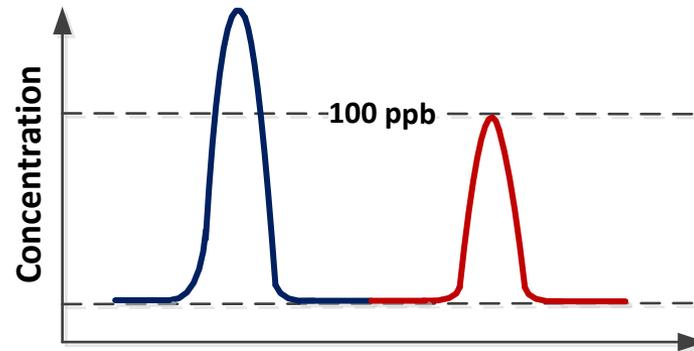
Surrogate Recovery = 100%

Analyte = 100 ppb



Surrogate Recovery = 25%

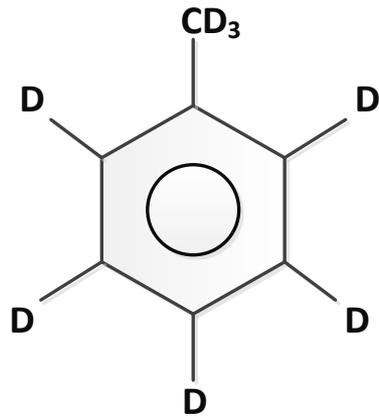
Analyte = 100 ppb



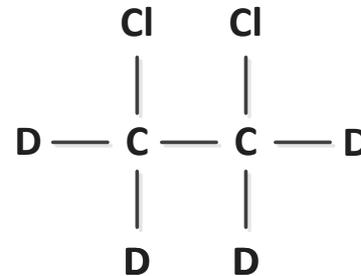
Surrogate Recovery = 150%

Analyte = 100 ppb

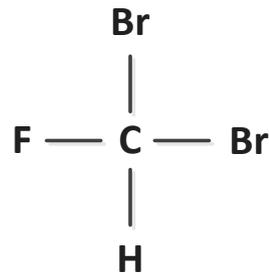
Surrogates for Volatiles by Method 8260B



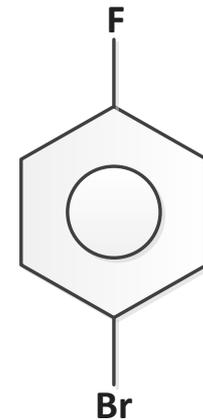
Toluene-d₈



1,2-dichloroethane-d₄



Dibromofluoromethane



4-Bromofluorobenzene

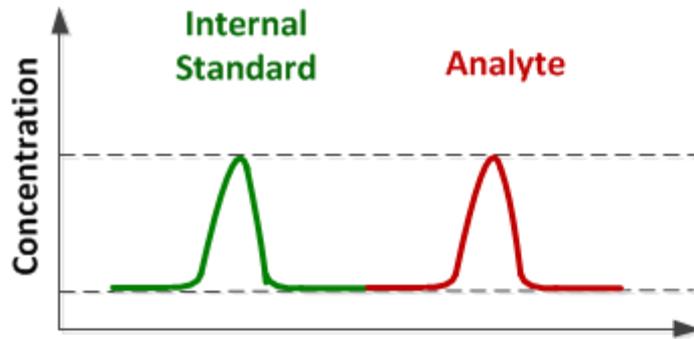
The Use of Internal Standards

Definition and Description of Use

Examples of Chemistry at Work

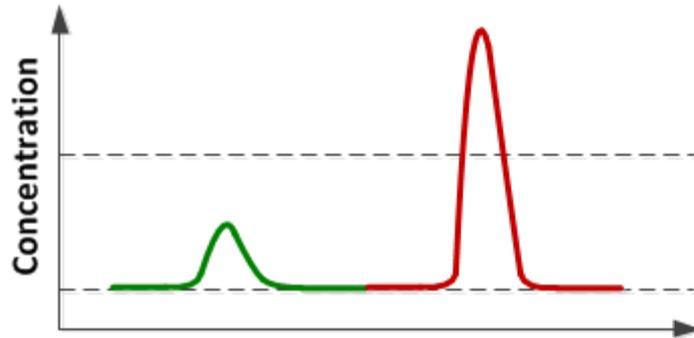
An internal standard is a compound that is chemically similar to analytes being determined and spiked directly onto a test sample at the analytical instrument used to perform the analytical test at a known concentration. The response of the instrument to the known level of internal standard is used to quantitate the analyte in the sample.

Internal Standard Spiked @ 100 ppb



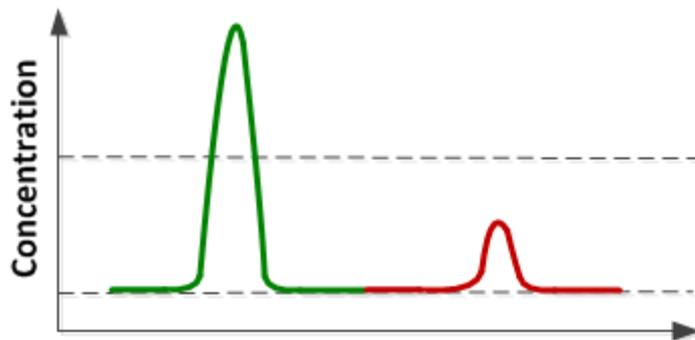
No Matrix Effects or 100% Recovery of the Internal Standard

Analyte has no apparent adjustment



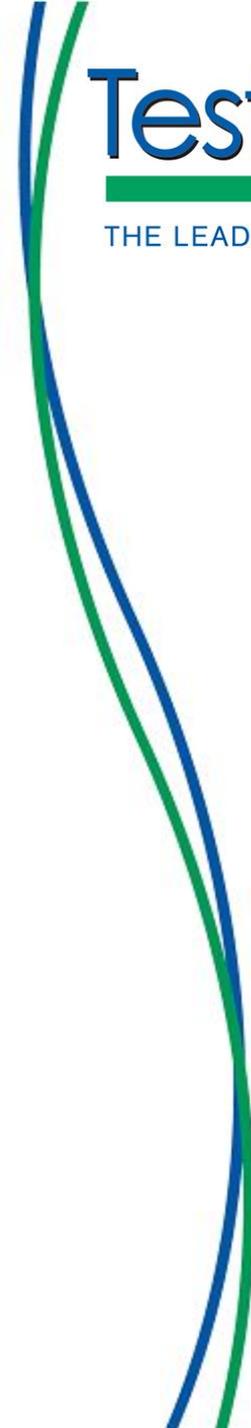
Matrix Suppressed Internal Standard

Analyte has apparent amplified concentration



Matrix Amplified Internal Standard

Analyte has apparent diminished concentration



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William C. Anderson, Ph.D.

Phone: (865) 291-3080

Website: testamericainc.com

Email: William.Anderson@testamericainc.com

**TestAmerica Laboratories, Inc.
5815 Middlebrook Pike
Knoxville, TN 37921**