

What is Mass Spectrometry?

Adapted from "What is Mass Spectrometry?"

by D.H. Chace and O.D. Sparkman, American Society for Mass Spectrometry, 2005

by
David C. Muddiman
and
Diana Ayerhart

Literature in Mass Spectrometry

Journal of the American Society for Mass Spectrometry

Rapid Communications in Mass Spectrometry

Journal of Mass Spectrometry

International Journal of Mass Spectrometry

European Journal of Mass Spectrometry

Mass Spectrometry Reviews

Analytical Chemistry

Journal of the American Chemical Society

Proceedings of the National Academy of Sciences

Journal of Chromatography

Journal of Proteome Research

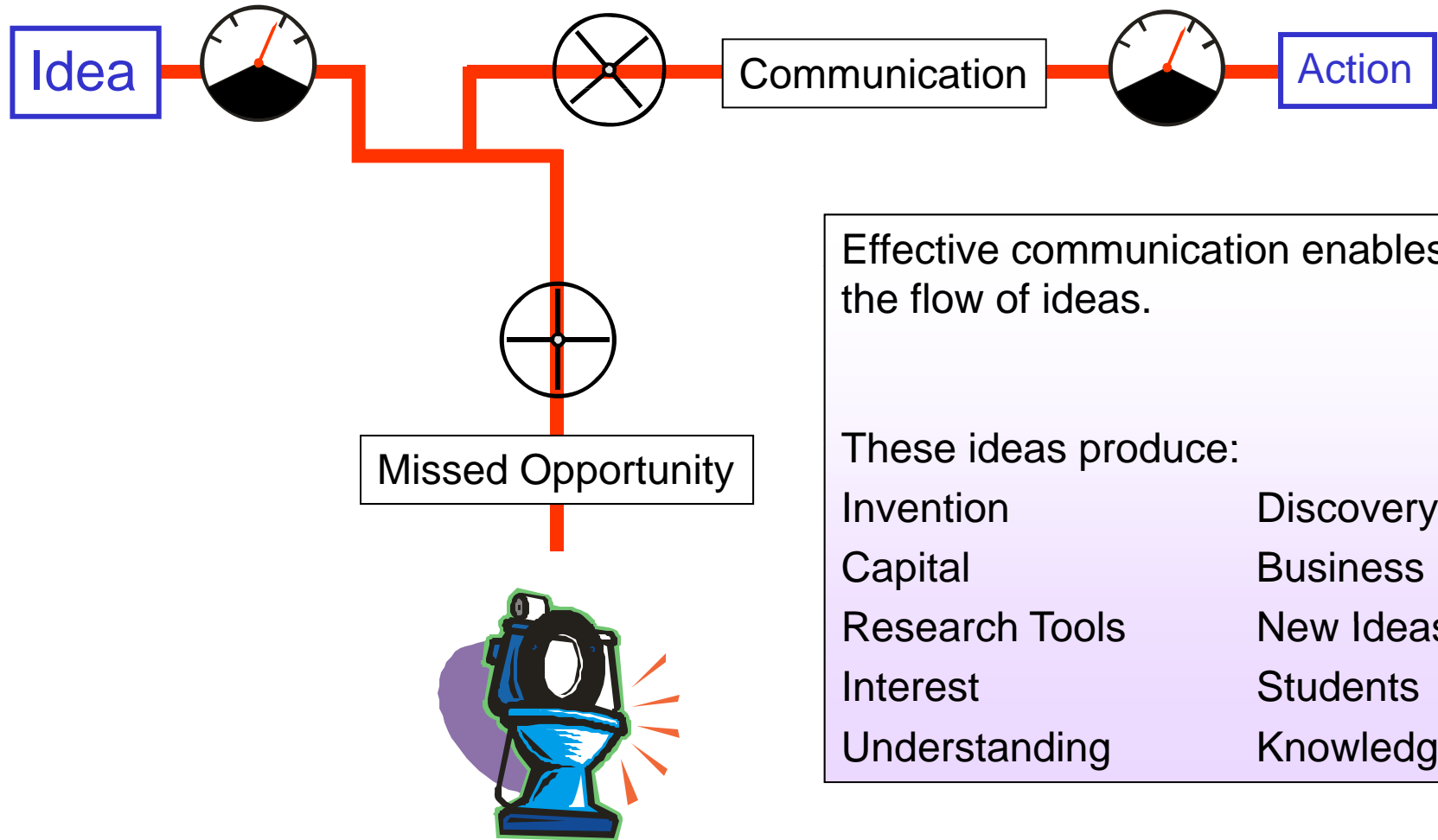
Electrophoresis

Journal of Biological Chemistry

Objective

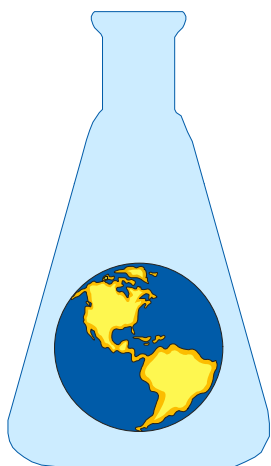
- To improve communication of mass spectrometrists with other professionals, media, and the educated consumer.
- To provide simple concepts, tools and resources to facilitate this communication.
- To initiate a serious discussion with regards to our role as mass spectrometrists to accomplish these goals.

Introduction



Statement of the Problem

Mass
Spectrometrists'
(Scientists)
View of the World



Mass Spectrometrists:

- fail to communicate impact of research
- others would not understand research
- narrow view versus integrated view

World's View of
Mass
Spectrometrists
(Scientists)



Public:

- disliked chemistry, wouldn't understand
- doesn't affect me
- doesn't need to know

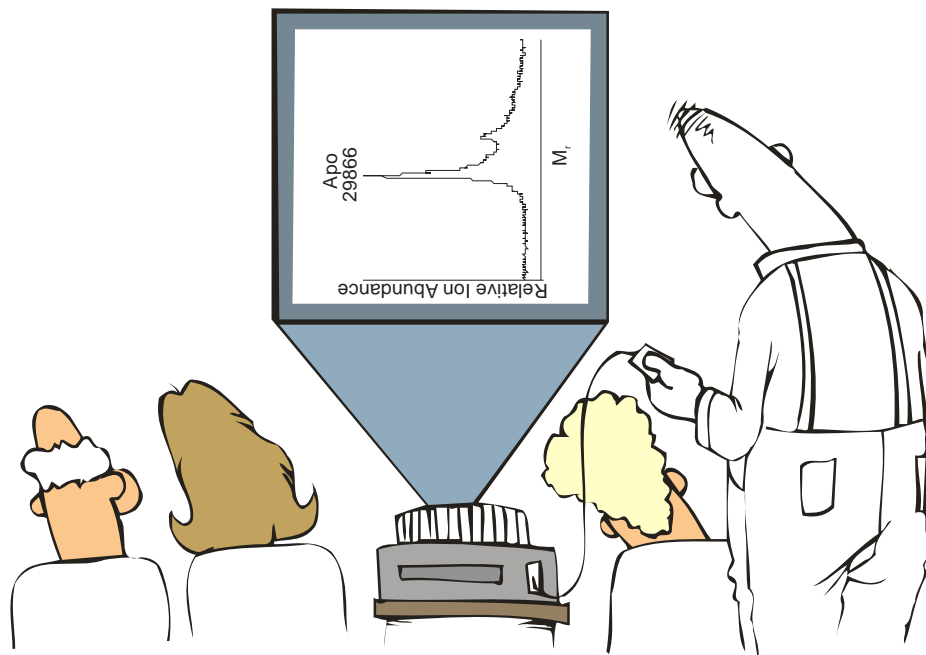
Solutions

Know your audience

- Mass spectrometrists, chemists
- Other scientists, professionals
- Educated consumer, media

Engage your audience

- Keep messages simple, direct.
- State the "bottom-line" repeatedly.
- Show why audience should care.
- Provide examples that the audience can relate to.



Utilize multiple forms of communication

- Supporting documents, brochures, handouts
- Multimedia (slide presentations, video)
- Internet (email, web pages)
- Press (printed, internet, digital, televised)

Team mass spectrometry

- Provide tools that can be shared
- Enhance education and outreach programs

Approach (Methods)

- Develop materials, illustrations, and instructional tools that can be shared within the MS community.
- Highlight limitations of current approaches and provide alternative examples.
- Use the model of Newborn Screening and Clinical Mass Spectrometry to highlight new approaches.

Concept 1: Mass Spectrometer

Mass Spectrometrists Definition:

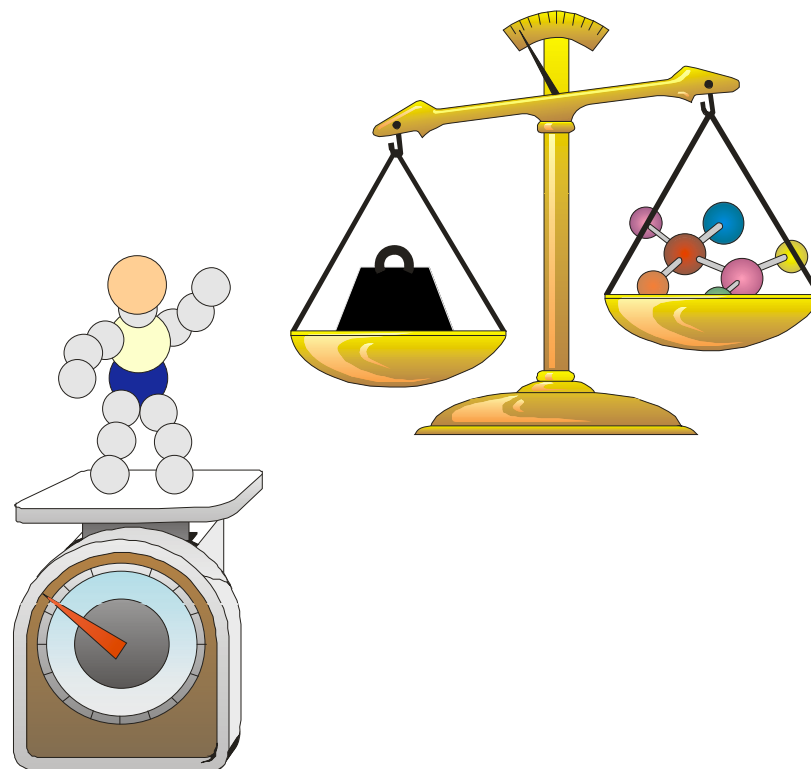
A mass spectrometer is an instrument that measures the masses of individual molecules that have been converted to ions; i.e., molecules that have been electrically charged.

Layperson Understanding:

The terms "masses" and "ions" may not be understood

Simple Definition:

A machine used to weigh molecules.
A molecular scale.



Concept 2: How is a mass spectrometer used?

Mass spectrometrists definition:

Mass spectrometry is a powerful technique that is used to identify unknown compounds, to quantify known materials, and to elucidate the structure and chemical properties of molecules.

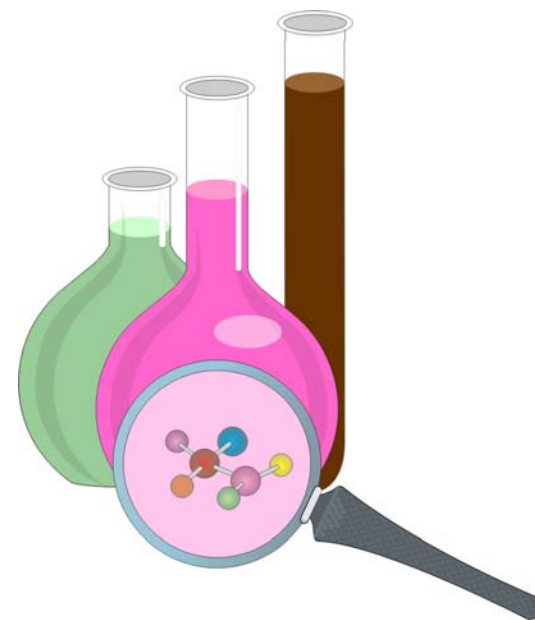
Layperson Understanding:

Powerful compared to what? Quantify? Elucidate?

Simple Definition

A mass spectrometer is used to help scientists:

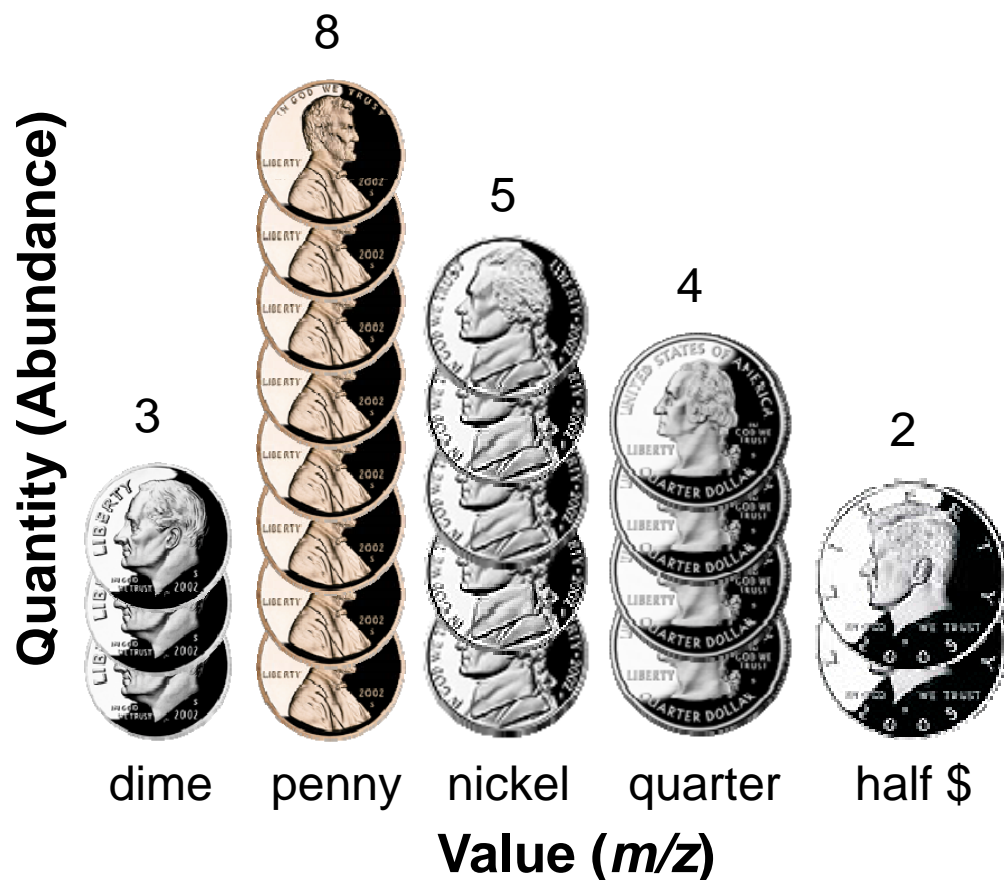
1. Identify molecules present in solids, liquids, and gases
2. Determine the quantity of each type of molecule.
3. Determine which atoms comprise a molecule and how they are arranged



Concept 3: Mass Analysis

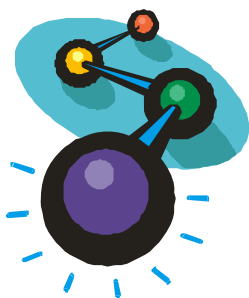
•Sorting and counting

- *Pocket change (mixture of coins)*
- *Penny, dime, nickel, quarter, half \$*
- *Sorting change by value or size*
- *Concept of visual interpretation*
- *Mixture of molecules*
- *Molecules of different weight, size*
- *Separation by mass spectrum*

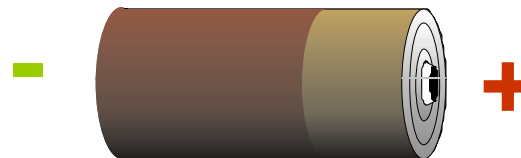


Concept 4: Ions and Charge

1. An ion is an electrically charged molecule.



2. An ion can be positively (+) charged or negatively (-) charged. Consider the poles on a battery.



3. Molecules must be charged to be measured by a mass spectrometer.

4. A mass spectrometer "weighs" molecules electronically by attracting and repelling ions. Consider magnets. Opposites attract. Like charges repel.



Concept 5: Ionization Techniques

Mass Spectrometrists Definitions:

Electrospray Ionization:
formation of charged liquid droplets from
which ions are desolvated or desorbed.

MALDI: (matrix-assisted laser desorption/ionization)
impact of high-energy photons on a sample
imbedded in a solid organic matrix.

Layperson Understanding:

None. How does this related to weighing molecules?

Simple Definition:

Ionization is a process of charging a molecule. Molecules must be charged in order to measure them using a mass spectrometer. "It makes a molecule fly in a mass spectrometer."

Electrospray



MALDI



Home – target, support
Dirt – compound
Paint – matrix
Pressurized water,
sand = laser

Concept 6: Tandem Mass Spectrometry

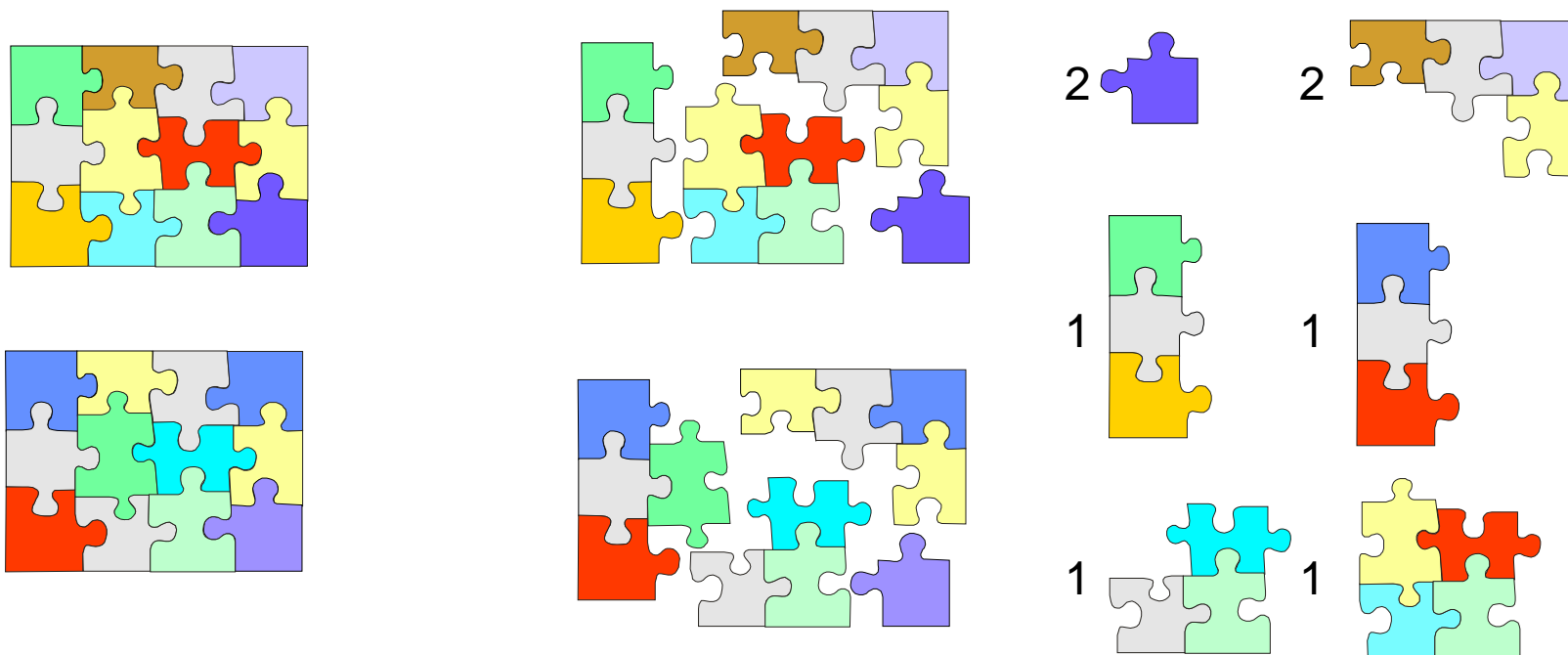
Simple Definition:

Two mass spectrometers joined by a chamber that breaks apart molecules.

This definition is appropriate for tandem-in-space but not for tandem-in-time.

Puzzle Analogy

MS #1	Fragmentation Chamber	MS #2
Sorting molecules	Breaking molecules	Sorting pieces



Concept 6: Tandem Mass Spectrometry

Word Analogy

Words

- Comprised of letters.
- Arrangement of letters gives words meaning.
- Special groups of letters make syllables.
- Common endings = suffixes.

Talk^{ing}

Writ^{ing}

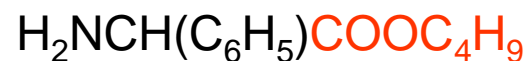
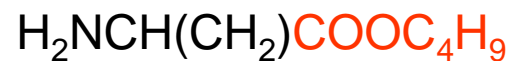
Play^{ing}

List all words containing "ing" in the book of abstracts

Use a computer to search for the string "ing" and it displays all words containing "ing".

Molecules

- Comprised of atoms.
- Arrangement of atoms gives molecules function.
- Special groups of atoms make functional groups.
- Common side chains = esters.



Detect all molecules containing a butyl formate functional group from an α -amino acid.

Use a NL scan function to detect only molecules that lose a butylformate function group weighing 102 Da

Concept 7: Quantification via IDMS

Simple Definition:

Isotope Dilution Mass Spectrometry (IDMS)

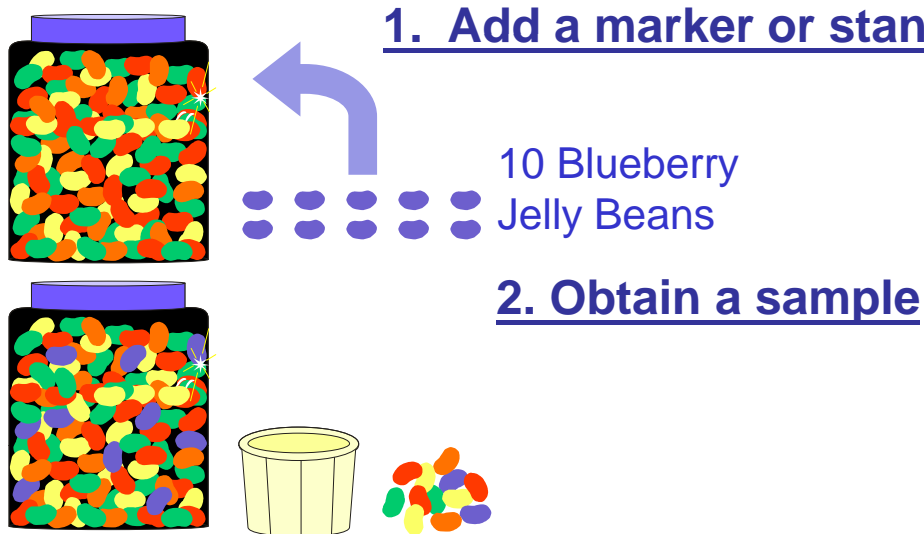
It is a method that measures how much compound X is present in a liquid, solid or gas.

This method uses non-radioactive elements called stable isotopes to make a comparison of compound X with the standard that contains the stable isotope. Since the amount of stable isotope standard is known, we can calculate how much compound X is present.

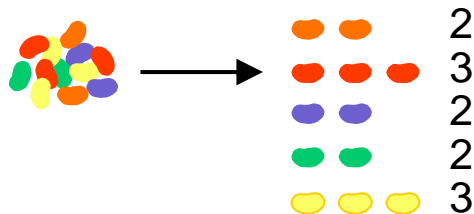
Jelly Bean Analogy

How many cherry jelly beans are in the jar?

How much phenylalanine is present in blood?

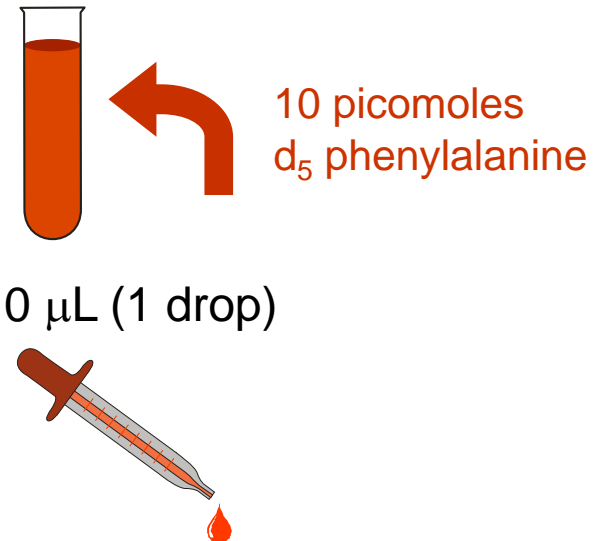


Sort jelly beans in the cup by flavor/color.
Count how many.

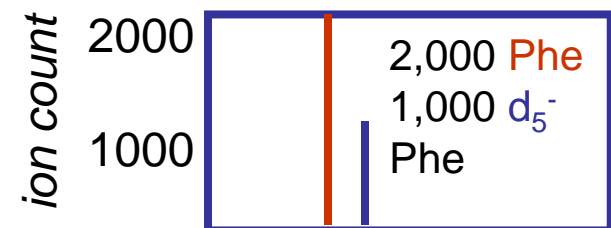


- 3 cherry w/ 2 blueberry in 1 oz
- $3/2$ ratio of cherry to blueberry
- 10 blueberry added to 1 oz
- $10 \times 3/2 = 15$
- 15 cherry red jelly beans in jar

3. Analysis



Sort phenylalanine by MS/MS
count how many



- 2,000 Phe, 1,000i.s.
- $2/1$ ratio of Phe to I.S.
- 10 pmol i.s. added to 1 mL blood
- $10 \times 2/1 = 20$ pmol
- 2- pmol Phe per mL of blood

Concept 8: Accuracy and Precision

Mass spectrometrists always say:

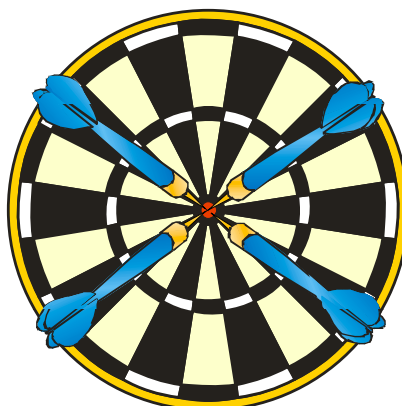
Mass spectrometry is very accurate and precise.

Reality:

Mass spectrometrists confuse accuracy and precision.

Dart Board Analogy

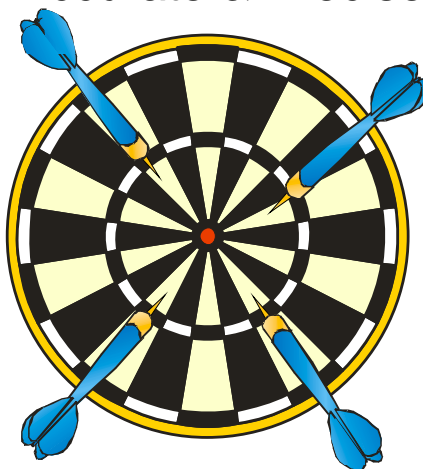
- Simple concept
- Visual
- Easily remembered
- Educational, fun



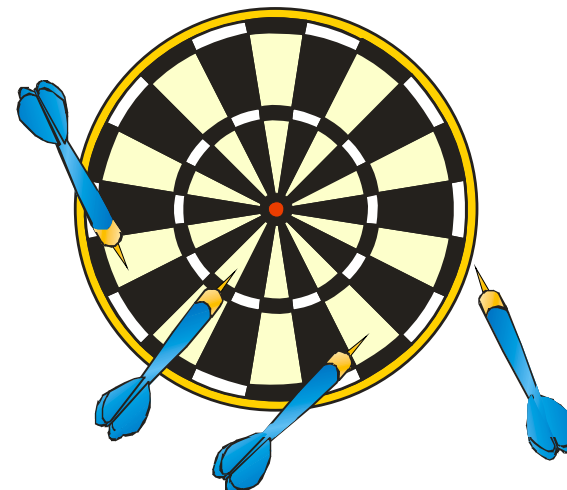
Accurate & Precise



Precise, Not Accurate



Accurate, Not Precise



Not Accurate, Not Precise

Summary

- Presented simple concepts, ideas that can foster other suggestions on communication.
- Mass spectrometry can be interesting, enjoyable, and fun.
- We need to develop more resources to support communication, especially with media, etc. Why? When a new method using MS to screen for ovarian cancer is called a computer method by the popular press, it is clear there is work to do!