Did you know…

that mass spectrometry is used to...

- Determine genetic diseases in newborns from blood spots
- Detect and identify the use of steroids in athletes
- Monitor the breath of patients by anesthesiologists during surgery
- Determine the composition of molecular species found in space
- Determine whether honey is adulterated with corn syrup
- Locate oil deposits by measuring petroleum precursors in rock
- Monitor fermentation processes for the biotechnology industry
- Detect dioxins in contaminated fish
- Determine gene damage from environmental causes
- Identify potentially pathogenic bacteria in the air
- Establish the elemental composition of semiconductor materials
- Detect explosives at airport security

2019 Galisteo St, Bldg I-1
Santa Fe, NM 87505
Telephone (505) 989-4517
Fax: (505)989-1073
E-mail info@asms.org
https://www.asms.org

Information, Web Links, Educational Resources

Comprehensive MS Information Resource
http://www.i-mass.com

Mass Spectrometry Links Resource
http://www.chemistry.gatech.edu/stms/links.html

Base Peak Links to Wiley Journals
http://base-peak.wiley.com/

Thomas Chasteen's GC/MS Movie
http://www.shsu.edu/%7Echm_tgc/sounds/GC-MS.mov

Fourier Transform Mass Spectrometry Tutorial
http://www.ionspec.com/FTMS%20Tutorial/FTMS%20Tutorial%20Home/tutorial%20hm_fs.htm

Peptide Mapping with MS/MS
http://www.mshri.on.ca/pawson/ms/ms.html

R. M. Jordan TOF Tutorial
http://www.rmjordan.com/tt1.html

Ion Trap Tutorial with a Bio Flavor
http://www.ionsource.com/links/iontrap.htm

Colby's Introduction to GC/MS
http://www.colby.edu/chemistry/OChem/DEMOS/MassSpec.html

Cambridge University Chemistry MS Tutorial
http://www-methods.ch.cam.ac.uk/meth/ms/theory/

An Introduction to Mass Spectrometry from Germany
http://www.ivv.fhg.de/ms/ms-introduction.html

JEOL Tutorials
http://www.jeol.com/ms/essays.html

FTICR Theory
http://www.emsl.pnl.gov/docs/msd/mass_spec/home/fticrtut.html#resonance

University of South Carolina GC-MS Methods
http://www.chem.sc.edu/analytical/chem723/gcmslab.html

University of Illinois
http://chipo.chem.uic.edu/web1/ocol/spec/MS1.htm

Moderated News Group
sci.techniques.mass-spec

Annual Mass Spectrometry Events

ASMS Annual Conference on Mass Spectrometry and Allied Topics (May/June)
Sanibel Conference (January)
Asilomar Conference (October)
ASMS Fall Workshop (November)
ASMS Short Courses on Different Aspects of Mass Spectrometry (May/June)

How to Use this Guide?

To the educator:

This poster was presented at the ASMS annual meeting in 2002 to openly discuss an important issue in science and specifically in mass spectrometry. Communication and understanding is extremely important in attracting students to the field of chemistry and science without intimidation or fear that may keep many bright students away. Scientists are uniquely challenged to present their data, discoveries, and tools in an easily understood format that would bring further interest, discovery, and funding to an important field of analytical and clinical chemistry. This poster is designed to show that science can be fun, interesting, and not something reserved for only the individuals with the highest IQ's. In fact, we need talent in writing, graphical arts, computer science, and law as we use a powerful new technology to solve many problems confronting the world today.

Suggestions:

1. *Assign students a class project of finding where a mass spectrometer is used today and describe this use.*

2. *Use some of these concepts such as accuracy, precision, and quantification to demonstrate that other studies such as math, statistics, physics, etc. are an essential part of the sciences.*

To the student:

1. *Enroll in a science fair and present a poster on one of the applications of mass spectrometry and show how it has improved our health, environment, or manufacturing processes.*

2. *Where have you seen Mass spectrometry applications in the media? Consider a "forensic science" investigation into a wrongful death or crime. How can MS be used to solve cause of death or provide clues at the scene of a crime?*

To the Business Professional:

1. *Learn the basic concepts and present them to colleagues, business associates to understand more about an important technology for the future so that wise investment and smart choices are made.*

What is Mass Spectrometry?

An Illustrated Guide To Mass Spectrometry

An educational tool for the introduction of mass spectrometry to the scientific professionals, media, students, and the general public

Donald H. Chace
O. David Sparkman
for the
American Society of Mass Spectrometry

What is Mass Spectrometry?

The Importance of Communicating the Concept of Mass Spectrometry to Professionals, Media, and the Consumer

*Donald H. Chace, O. David Sparkman, *Pediatrix Analytical, Bridgeville, PA, and University of the Pacific, Stockton, CA

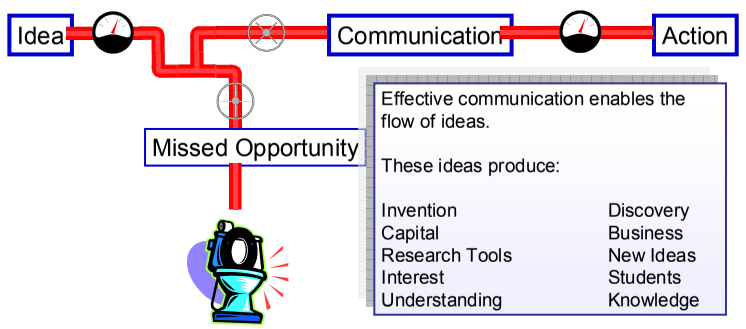
Objective

➢ 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

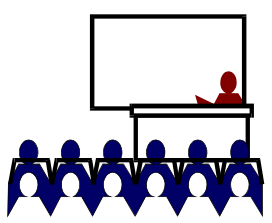
Mass Spectrometrists:
- fail to communicate impact of research
- others would not understand research
- narrow view versus integrated view

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, 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 Spectrometrist 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, ions may not be understood.

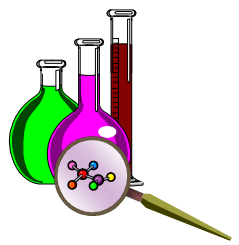
Simple Definition:
A machine used to weigh molecules.
A molecular scale.

Concept 2: How is a mass spectrometer used?

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

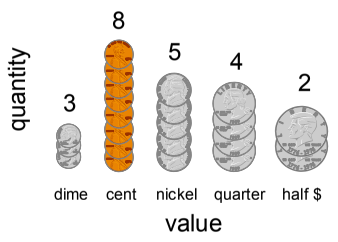
Layperson Understanding:
Powerful compared to what? Quantify? Elucidate?

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

[1]Mass Spectrometrist Definitions:

Electrospray: *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 relate 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

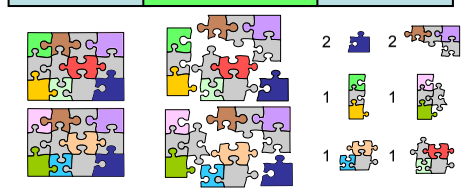
Home – target, support
Dirt – compound
Paint – matrix
Pressurized Water, Sand – Laser

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*



- Word Analogy

Words	Molecules
Comprised of letters.	Comprised of atoms.
Arrangement of letters gives words meaning.	Arrangement of atoms gives molecules function.
Special groups of letters make syllables.	Special groups of atoms make functional groups.
Common endings = suffixes.	Common side chains = esters
Talking Writing Playing	$H_2NCH_2COOC_4H_9$ $H_2NCH(CH_2)COOC_4H_9$ $H_2NCH(C_6H_5)COOC_4H_9$

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."

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.

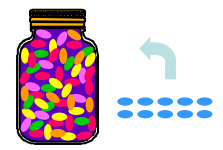
Concept 7: Quantification via IDMS

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.

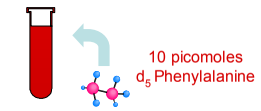
- Jelly Bean Analogy

How many Cherry Jelly Beans are in the jar? *How much phenylalanine is present in Blood*

1. Add a marker or standard



10 Blueberry Jelly Beans



10 picomoles d_5 Phenylalanine

2. Obtain a sample.

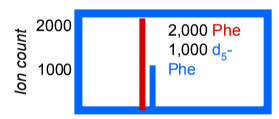
1 oz

10 uL (1 drop)

3. Analysis.

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

Sort Phenylalanine by MS/MS
Count how many.



3. Calculations

a.) 3 Cherry Red, 2 Blueberry in 1 oz
b.) 3/2 ratio of Cherry to Blueberry
c.) 10 Blueberry added to 1 oz.
d.) 10 x 3/2 = 15
e.) 15 Cherry Red Jelly Beans in Jar

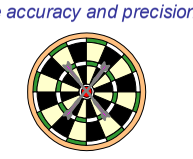
a.) 2,000 Phe, 1,000 i.s.
b.) 2/1 ratio of Phe to I.S.
c.) 10 pmol i.s. added to 1 mL blood
d.) 10 x 2/1 = 20 pmol
e.) 20pmol Phe per mL of blood

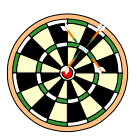
Concept 8: Accuracy and Precision

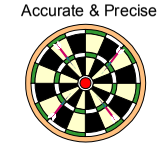
Mass Spectrometrists always say:
Mass Spectrometry is very accurate and precise.

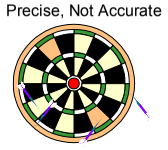
Reality:
Mass Spectrometrists confuse accuracy and precision.

- 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.*