MINNESOTA CHROMATOGRAPHY FORUM

Introduction to Mass Spectral Interpretation

by Robert Kobelski

Each mass spectrum contains a wealth of information. With higher resolution instruments, faster computers, larger and better spectral libraries, and more reliable comparison algorithms some will contend identification of an unknown compound from its mass spectrum is both unambiguous and completely automated. The tools available today make qualitative mass spectrometry easier and more reliable than ever before but a thorough understanding of how to exploit the information in a mass spectrum becomes critical to confirm the results of a library search and becomes more important when there is no good match in the library database as is the case for many spectra produced by soft ionization techniques and collision induced dissociation.

This course will explore the chemical information present in a mass spectrum and how to use this information to propose possible molecular structures consistent with the spectral information. The focus will be on the use of stable isotope information to assist with the determination of a molecular formula and the use of logical losses, both radical and neutral molecule, to assist with assigning possible structures.

Course Outline

Day 1

1. Introduction & Information Content of a Mass Spectrum
    a. Atomic “weight”
    b. Molecular “weight”
    c. Mass Resolution
    d. Isotopic Information
    e. Molecular fragmentation
2. Ionization Processes
    a. Odd and even electron ions
    b. Electron Ionization (EI)
    c. Chemical Ionization (CI & APCI)
    d. Electrospray Ionization (ESI)
    e. MALDI
3. “A” Elements (Mono-isotopic Elements)
4. “A+1” Elements (Carbon & Nitrogen)
    a. Isotopic Abundances
    b. Nitrogen Rule
5. Logical Losses
    a. Radical Losses
    b. Molecular losses
6. MS Library Searching

Day 2

7. Review of Day 1
8. Ion Stability
    a. Structure/Stability
    b. Stability/Abundance
    c. Stevenson's Rule
9. Single "A+2" Elements
    a. Chlorine
    b. Bromine
    c. Silicon
    d. Sulfur
10. Multiple "A+2" Elements
    a. Pattern Recognition
    b. Calculating Distributions
11. Accurate Mass & Elemental Composition

Sessions 3, 4, 7, 9 and 10 contain imbedded problems and exercises

Robert Kobelski, PhD

Bob Kobelski, Lead Chemist, serves as the Laboratory Chief of the Laboratory Response Network for Chemical Threats (LRN-C). In this capacity, Dr. Kobelski provides guidance and leadership for a network of 54 emergency response labs located in public health laboratories across the country. Before assuming his current role, Dr. Kobelski was a Research Chemist in DLS's Volatile Organic Compounds Laboratory. Previously, Dr. Kobelski worked in the private sector in the following capacities: chemist (Dupont), senior analytical research chemist (Buffalo Color Corporation), senior research chemist/principal scientist (Johnson and Johnson Personal Products Company), applications engineer/consultant (Hewlett-Packard, Analytical Product Group), manufacturing/hardware design engineer (Hewlett-Packard, Inkjet Supplies Business Unit), and director of analytical chemistry (MetaMetrix Clinical Laboratory).

Dr. Kobelski obtained his doctorate in analytical chemistry from the State University of New York at Buffalo in 1986. He obtained his master's degree in organic chemistry from the University of Vermont in 1973 and his bachelor's degree in chemistry from Fordham University in 1970. He began teaching MS interpretation classes in the previous millennium and continues to expand and refine the course material as mass spectrometry evolves.