Interpretation of Mass Spectra

Agilent Chemical Analysis Training Courses

H4063A

Three Days
Lecture Only

Description

Presents the fundamental concepts necessary to obtain high-quality data in SCAN mode from a gas chromatograph-mass spectrometer (GC-MS) system. Such data quality is essential for accurate spectral interpretation.

Introduces the most commonly used tools for identifying compounds based on their mass spectra and explains the physical reasons for the effectiveness of these tools.

Also covers the most common decomposition mechanisms responsible for fragment ions in mass spectra. These mechanisms can help determine an appropriate structure from among a number of possible isomers.

Problem-solving exercises reinforce instruction.

This course provides a more comprehensive introduction to mass spectral interpretation than Introduction to Mass Spectral Interpretation I and II (H5313A and H5319A).

2.4 CEUs

Course Outline

Day One

- GC-MS Data Structure
- Chemistry Review
- Data Acquisition

Day Two

- Introduction to Interpretation Goals
- Structural Information
- Spectrum Appearance
- Elemental Composition
- Use of Isotopic Abundance
- Rings and Double Bond Calculations
- Deducing Elemental Composition

Day Three

- The Molecular Ion
- Nitrogen Rule
- Logical and Illogical Neutral Losses
- Abundance versus Ion Structure
- Library Searching

Prerequisites

Undergraduate training in organic chemistry and at least six months of experience in obtaining spectra with a modern mass spectrometer and data system.

Students should bring a calculator to aid problem solving.

Student Profile

An advanced GC-MS operator or GC-MS supervisor responsible for identifying unknown spectra or evaluating MS library database search results.

Equipment Used during Training

Lecture only

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