



GC-MS Data Interpretation

This course provides the basic knowledge required for the interpretation of unknown spectra. Starting from the first principles, it introduces the fundamental chemistry of mass spectrometry and builds up to an examination of the most frequently encountered fragmentation patterns.

This course is not instrument-specific and is suitable for anyone involved in mass spectrometry. A good working knowledge of the technique is required and attendance on our "GC/MS for the chromatographer" course is recommended prior to attendance on this course.

Course Contents

Basic Chemistry

- Review of the chemistry of ions, electrons and radicals and isotopes vital to understanding of molecular fragmentation and ionisation
- The principles of isotopic normalisation

Principles of Ionisation

- Techniques and impact on ionisation and fragmentation of Electron Impact (EI) and Chemically Induced (CI) ionisation mechanisms

Fragmentation Mechanisms

- Homo and heterolytic fission
- Alpha cleavage
- Inductive cleavage
- McLafferty rearrangement and ortho effects
- Retro Diels-Alder reactions

Interpretation Rules

- General appearance
- Isotopic abundances
- Isotopic normalisation
- Common ion series
- Rings and double bonds
- The nitrogen rule
- Logical (Illogical) neutral molecular losses
- Logical (Illogical) neutral fragment losses
- Ion stability

Interpretation Practice

- At all points during the course, practice spectra are given to highlight and allow the student to learn the principles under investigation
- The course ends with practice exercises on several spectra to confirm overall understanding



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