

LC-MS Data Interpretation

Attendees on this courses will benefit from a greater understanding of how to interpret the mass spectra produced by Electrospray Ionisation (ESI) and Atmospheric Pressure Chemical Ionisation (APCI).

This course will give the delegate increased confidence and understanding of:

- Mass spectral data analysis
- Structural elucidation
- Product ion generation by Collision Induced Dissociation (CID) characterization
- Advantages and limitations of common mass analyser types

Course Contents

Interpretation of low molecular weight compound mass spectra considers the importance of:

- Understanding isotope patterns and their relative signal responses in assigning elemental composition and confirming chemical structure
- Understanding how common characteristic production fragmentation series are produced through atomic electronic effects
- A mechanistic understanding of the inductive and alpha cleavage
- How CID fragmentation can be invaluable for sample identification purposes through first principles interpretation and database searching
- Inclusion of peptide sequencing by tandem mass spectrometry as required

Interpretation of high molecular weight compound mass spectra considers the importance of:

- When to report monoisotopic mass or average mass
- The process of deconvolution of an ESI multiply charged ion series to derive the molecular weight of a compound

Further

- Explanation of the formation of common adduct ions under different solvent and buffer conditions
- Solution and source compound dimerisation effects
- The process of data dependent acquisition and modern detector systems
- Comprehensive set of tutor-led tutorial questions to facilitate the learning process

