

# CH908-10 Mass Spectrometry

**26/27**

**Department**

Chemistry

**Level**

Taught Postgraduate Level

**Module leader**

Peter O'Connor

**Credit value**

10

**Module duration**

2 weeks

**Assessment**

50% coursework, 50% exam

**Study location**

University of Warwick main campus, Coventry

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## Description

### Introductory description

This module introduces the student to the many facets of modern mass spectrometry. Emphasis is placed both on the interpretation of spectra and also on instrumental methods, covering modern methods of ionisation (including ESI and MALDI) and mass analysis (including orthogonal TOF and FT-ICR) and the use of linked methods such as GC/MS, HPLC/MS and tandem mass spectrometry. Practical sessions include practice at interpretation and experiments using various mass spectrometric techniques.

[Module web page](#)

### Module aims

To introduce students to the physical and instrumental basis of mass spectrometry, and to enable them to interpret mass spectra from a variety of ionisation techniques.

### Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be covered. Actual sessions held may differ.

1. Principle of a mass spectrometer. EI and CI. Isotopic pattern.
2. Molecular ion region to elucidate elemental composition. Nitrogen rule. Odd. vs. Even electron ions and their spectra. Neutral losses.
3. Fragmentation pattern of important compound classes in EI. McLafferty rearrangement, cleavages, etc. Composition of structure through analysis of fragmentation pattern.
4. Standard Odd- and Even- electron fragmentation chemical principles and rearrangements. Examples of such.
5. Principles of Matrix-assisted Laser Desorption/Ionisation (MALDI)
6. Principles of Electrospray Ionisation (ESI)
7. Polymer mass spectrometry, high resolution analyses, elemental composition analysis, and other uses of MS that don't require MS/MS.
8. Introduction to mass analyzers, Details of the quadrupole mass analyzer.
9. Details of the modern Time-of-Flight analyser, FTICR mass analyzer, Orbitrap.
10. MS/MS methods, focusing on CAD and IRMPD, and related methods
11. MS/MS methods, focusing on ECD, ETD, and related methods.
12. Protein and peptide MS/MS, sequencing peptides
13. Protein and peptide MS/MS, identifying PTMs
14. Modern proteomics
15. Other biomolecules.

The formal lectures will be supplemented by several class exercises/examples to reinforce the lecture material (also available to other postgraduates), plus five full practical laboratory sessions. The course does NOT need prior knowledge of MS, but does require a basic understanding of general chemistry and organic chemistry at an undergraduate level. The practicals include live MALDI and ESI sessions, EI/CI and GCMS sessions, at least one proteomics session, and experience dealing with data from a variety of different mass analyzers.

## Learning outcomes

By the end of the module, students should be able to:

- Students will have acquired knowledge and understanding in modern mass spectrometry, and will be able to handle and analyse MS data.
- Interpret EI mass spectra in order to elucidate elemental composition and structure of basic organic compounds
- Have a good understanding of the physical principles used in mass spectrometry
- Detailed understanding of modern ionisation methods (“soft” ionisation)
- Understanding of the use of modern MS in current research regarding material and biological sciences
- Good understanding of electrospray and Matrix-assisted laser desorption mass spectra of peptides, and their uses in 1) identifying proteins, 2) sequencing peptides and proteins, and 3) determining post-translational modifications. How to use these spectra in proteomics experiments.

## Indicative reading list

## Subject specific skills

Interpret EI mass spectra in order to elucidate elemental composition and structure of basic organic compounds

Have a good understanding of the physical principles used in mass spectrometry

Detailed understanding of modern ionisation methods ("soft" ionisation)

Familiarity with different types of mass analysers and sound understanding of time-of-flight Mass Spectrometry, quadrupoles, and Fourier-Transform Ion Cyclotron Resonance Mass analysers

Understanding of the use of modern MS in current research regarding material and biological sciences

Good understanding of electrospray and Matrix-assisted laser desorption mass spectra of peptides, and their uses in 1) identifying proteins, 2) sequencing peptides and proteins, and 3) determining post-translational modifications. How to use these spectra in proteomics experiments.

## Transferable skills

### 1 Critical thinking

- Recognise patterns, themes and key messages from sometimes confused and incomplete data.
- Make informed decisions on the value of a range of sources allowing an evidence based conclusion based on this analysis.

### 2 Problem solving

- Use rational and logical reasoning to deduce appropriate and well-reasoned conclusions.
- Retain an open mind, optimistic of finding solutions, thinking laterally and creatively to look beyond the obvious.
- Knows how to learn from failure.

### 3 Self-awareness

- Actively seek opportunities for personal development in the context of employment and life.
- Aware of personal strengths and emotional intelligence
- Reflect on learning, seeking feedback on and evaluating personal practices, strengths and opportunities for personal growth.

### 4 Communication

- Communicate orally in a clear and sensitive manner which is appropriately varied according to different audiences.
- Written: Present arguments, knowledge and ideas, in a range of formats. Active listening: questioning, reflecting, summarising.

### 5 Teamwork and working effectively with others

- Operate within, and contribute to, a respectful, supportive and cooperative group climate.
- Sensitive to the impact of actions on others.

### 6 Information literacy (research skills)

- Critical awareness of how information is gathered, used, managed and synthesised.
- Understanding of the relative value of different sources and the importance of provenance.
- The systematic collection, analysis and evaluation of information in the investigation of a topic.

### 7 Digital literacy

- Has the capabilities that enable living, learning and working in a digital society.
- Comfortable with using digital media to communicate, solve problems, manage information, collaborate, create and share content.

### 8 Sustainability

- Understands the climate emergency and committed to an active contribution to a sustainable world.

### 9 Ethical values

- Committed to living ethically and behaving consistent with the Warwick Guiding Principles.

### 10 Intercultural awareness

- Develop required observational, analytical and reflection skills to understand impact of culture on self and on interactions with culturally different others.
- Demonstrating a curiosity, spirit of adventure and willingness to take risks in the pursuit of increasing intercultural knowledge and sensitivity.

### 11 Professionalism

- Prepared to operate autonomously.
- Aware of how to be efficient and resilient.
- Manages priorities and time.
- Self-motivated, setting and achieving goals, prioritising tasks.

### 12 Organisational awareness

- Understanding of business, government and third sector issues and priorities.
  - Awareness of the responsibilities of organisations in society.
  - Understanding organisational norms of behaviour
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## Study

### Study time

Type	Required
Lectures	8 sessions of 2 hours (16%)
Practical classes	7 sessions of 4 hours (28%)
Supervised practical classes	1 session of 6 hours (6%)
Private study	50 hours (50%)
Total	100 hours

### Private study description

50 hours independent revision

### Costs

No further costs have been identified for this module.

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## Assessment

You do not need to pass all assessment components to pass the module.

### Assessment group C6

	Weighting	Study time	Eligible for self-certification
<b>Assessment component</b>			
Written Assessments written reports, 5 pages each	50%		Yes (extension)
<b>Reassessment component is the same</b>			
<b>Assessment component</b>			
Written Examination (Locally Held) Standard written exam	50%		No
<b>Reassessment component is the same</b>			

### Feedback on assessment

Marked homework sets will be returned within 20 working days.

[Past exam papers for CH908](#)

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## Availability

### Courses

This module is Optional for:

- Year 1 of TCHA-F1PY Postgraduate Taught Analytical Science and Instrumentation
- Year 1 of TCHA-F1PX Postgraduate Taught Analytical and Polymer Science
- Year 1 of TCHS-F1PK Postgraduate Taught Polymer Chemistry
- Year 1 of TCHA-F1PW Postgraduate Taught Polymer Science