CH3F2-15 Advanced Analytical Chemistry

21/22

Department
Chemistry
Level
Undergraduate Level 3
Module leader
Mark Barrow
Credit value
15
Module duration
15 weeks
Assessment
33% coursework, 67% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

n/a.

Module web page

Module aims

This Core module focuses on theoretical and practical aspects of instrumental analytical techniques, including data generation, acquisition, processing, and interpretation, instrumentation and state-of-the-art applications. A range of techniques will be considered with emphasis being placed on chromatography, mass spectrometry, and nuclear magnetic resonance spectroscopy.

Techniques covered in lectures are reinforced in laboratory and workshop sessions.

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.

Chromatography

- Chromatography theory
- Gas chromatography principles and practice
- Liquid chromatography principles and practice including thin layer chromatography, colum chromatography and high performance liquid chromatography (HPLC), including normal phase, reverse phase, and chiral chromatography. Hyphenated techniques including chromatography

Mass Spectrometry

- Basic terminology and concepts, including measures of performance
- Methods of producing ionized samples for mass spectrometry including: electron ionization (EI), matrix-assisted laser desorption/ionization (MALDI), electrospray ionization (ESI), and atmospheric pressure photoionization (APPI)
- Different types of analyzers including: time-of-flight, quadrupole mass analyser, Fourier transform ion cyclotron resonance, and Orbitrap
- Tandem mass spectrometry (MS/MS) techniques, such as collision-induced dissociation (CID)
- Analysis of mass spectra, including calculating masses using charge states or isotopic distributions; use of online protein databases
- Advanced data visualization methods, such as Kendrick mass defect plots
- Hyphenated techniques such as GC-MS or LC-MS
- Quantitation of analytes
- Proteomics
- Polymer analysis

Nuclear magnetic resonance spectroscopy

- Theoretical concepts of NMR including energy levels, magnetisation, radio frequency pulses, role of nuclear spin.
- Principles of continuous wave NMR and of Fourier Transform NMR including magnetisation, effect of RF pulse, physical basis of relaxation, NMR timescales, NMR lifetimes, nature of T1 and T2, line-widths, anisotropy.
- Consideration of NMR active nuclei including quadrupolar nuclei
- Solid-state NMR
- Introduction to EPR
  Advanced NMR techniques and their applications:
- 2D NMR: Including COSY, TOCSY, NOESY
- Polarisation transfer
- Carbon NMR
- A selection of other NMR techniques

Laboratory/workshop
Students will undertake a number of data handling and analysis laboratory workshops. Practicals will involve data acquisition (MRI, MS, NMR, Chromatography, IR, UV and elemental analysis techniques), with emphasis on high quality data collection and interpretation. Students will also undertake a project to determine the identity of an unknown compound. They will choose which techniques are most appropriate to use, process data using proprietary software all within a given

financial budget and provide a written report on the analysis.

Learning outcomes

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

- Subject knowledge and understanding: Show an understanding of the fundamental principles behind analytical and spectroscopic methods and functions of various components in complex spectroscopic instrumentation; Appreciate Instrument performance characteristics; Demonstrate ability to process outputs from analytical instruments into interpretable datasets; Demonstrate the ability to evaluate and interpret data from a variety of measurements; Display consideration for sources and treatment of experimental error
- Key Skills: Demonstrate numeracy; Independently use information technology: databases, data-processing and other software.
- Cognitive Skills: Critically analyse data; Comprehensively assess errors in data; Test hypotheses using experimental data
- Subject-Specific/Professional Skills: Demonstrate sound laboratory and measurement skills; Follow good and safe practice in the laboratory.
- Demonstrate good team working
- Demonstrate financial budgeting
- Demonstrate timely planning of laboratory schedule
- Demonstrate ability to determine which experiments are necessary/unnecessary to provide desired outcome

Indicative reading list

Holler, Skoog, Crouch, Principle of Instrumental Analysis, 6th Edition.
Dudley H. Williams, Ian Fleming, Spectroscopic methods in organic chemistry.
Akitt and Mann, NMR and Chemistry
McLafferty and Turecek, Interpretation of Mass Spectra, 4th ed.
“Mass Spectrometry” by James McCullagh and Neil Oldham, Oxford Chemistry Primers
“Mass Spectrometry: Principles and Applications” by Edmond de Hoffmann and Vincent Stroobant, Wiley
“Mass Spectrometry: A textbook” by Jürgen Gross, Springer

Research element

e.g. individual or group research, research skills activity, etc.

Subject specific skills

Numeracy
Critical thinking
Information literacy and research skills

Transferable skills

Numeracy
Critical thinking
Information literacy and research skills

Study

Study time

Type	Required	Optional
Lectures	20 sessions of 1 hour (13%)	3 sessions of
Practical classes	10 sessions of 1 hour (7%)	
Private study	120 hours (80%)	
Total	150 hours	

Private study description

N/A

Costs

No further costs have been identified for this module.

Assessment

You must pass all assessment components to pass the module.

Students can register for this module without taking any assessment.

Assessment group D2

Assessment component	Weighting	Study time	Eligible for self-certification
Laboratory project (pair/group work)	33%		No

AIM: To work in a team and experience a real-life research style analytical problem while carrying out appropriate analytical experiments determined by the team. You need to keep the costs of your research to a minimum, efficiently assign roles and tasks to team members and to write a report of your findings in a predetermined format. As this is a research project you will need to

	Weighting	Study time	Eligible for self-certification

work independently and find solutions to questions yourselves within your team. This will be assessed by a joint team report (80%) plus an individual self-reflection document and a joint team self-reflection document and task log (20%).

Reassessment component is the same

Assessment component

Online Examination	67%		No

Examination on chromatography, mass spectrometry, and NMR lectures.

~Platforms - AEP

- Answerbook Green (8 page)
- Students may use a calculator
- Periodic Tables

Reassessment component is the same

Feedback on assessment

Written feedback on workshops from assessor. Cohort level examination feedback provided via Moodle.

Past exam papers for CH3F2

Availability

Pre-requisites

To take this module, you must have passed:

- All of
  - CH222-30 Practical and Professional Chemistry Skills II

Courses

This module is Core for:

- UCHA-4 Undergraduate Chemistry (with Intercalated Year) Variants
  - Year 4 of F101 Chemistry (with Intercalated Year)
  - Year 4 of F122 Chemistry with Medicinal Chemistry (with Intercalated Year)
- UCHA-3 Undergraduate Chemistry 3 Year Variants
  - Year 3 of F100 Chemistry
  - Year 3 of F121 Chemistry with Medicinal Chemistry
- Year 3 of UCHA-F110 Undergraduate Master of Chemistry (with Industrial Placement)
- Year 4 of UCHA-F107 Undergraduate Master of Chemistry (with Intercalated Year)
- UCHA-F109 Undergraduate Master of Chemistry (with International Placement)
  - Year 3 of F109 MChem Chemistry (with International Placement)
  - Year 3 of F111 MChem Chemistry with Medicinal Chemistry (with International Placement)
- UCHA-4M Undergraduate Master of Chemistry Variants
  - Year 3 of F100 Chemistry
  - Year 3 of F105 Chemistry
  - Year 3 of F109 MChem Chemistry (with International Placement)
  - Year 3 of F126 MChem Chemistry with Med Chem (with Prof Exp)
  - Year 3 of F125 MChem Chemistry with Medicinal Chemistry
  - Year 3 of F106 MChem Chemistry with Professional Experience
- Year 4 of UCHA-F127 Undergraduate Master of Chemistry with Medicinal Chemistry(with Intercalated Year)