CH921-10 Frontier Techniques in Analytical Science

24/25

Department
Chemistry
Level
Taught Postgraduate Level
Module leader
Claudia Blindauer
Credit value
10
Module duration
10 weeks
Assessment
50% coursework, 50% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

To introduce students from a range of different backgrounds to advanced analytical techniques. To ensure students appreciate the links between need for measurement, instrumentation design, data quality and data analysis.

Module web page

Module aims

To introduce students from a range of different backgrounds to advanced analytical 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.

- Importance of and areas of applications of qualitative/quantitative analyses
- Experimental error

- Volumetric and gravimetric methods
- Optical spectroscopy:
  o Absorption, emission, fluorescence
  o Atomic and molecular spectra
  o Spectrophotometry
- Infrared spectroscopy
- Atomic spectroscopies/Elemental Analysis: Fundamentals, instrumentation, and applications of
  o Atomic absorption spectroscopy (AAS)
  o Atomic emission spectroscopy (AES)
  o Inductively coupled plasma spectroscopy (ICP)
- X-ray spectroscopy:
  o Absorption
  o Fluorescence
  o Diffraction
- Nuclear Magnetic Resonance:
  o Foundations of Nuclear Magnetic Resonance (NMR), e.g., spin angular momentum, Larmor frequency, instrumentation requirements, NMR interactions: chemical shifts, J and dipolar couplings, quadrupolar, Fourier transformation).
  o Basic concepts in solid-state NMR (magic-angle spinning, cross polarisation, 2D methods, applications to, e.g., pharmaceuticals).
- Circular and linear dichroism: spectroscopic principles, relationship of measured signals to molecular structure, sample preparation, instrument design, data collection and analysis.
- Raman Spectroscopy: spectroscopic principles, instrument design options, relationship of measured signals to molecular structure
- Surface Spectroscopies:
  o X-Ray Photoemission Spectroscopy (XPS)
  o Infrared Reflection Adsorption Spectroscopy (IRRAS)
  o Secondary Ion Mass Spectrometry (SIMS)
- Electrochemical sensors:
  o Fundamentals of electrochemical sensors
  o Scope of electrochemical sensor applications – from clinical diagnostics to environmental sensing
  o Integrated sensor systems, including functionalised interfaces
  o Frontiers in electrochemical sensing – new electrode materials, single molecule detection, nanoscale imaging, cheap (paper-based) platforms, microfluidics
- Mass spectrometry
  o Instrumentation
  o Mass Analysers: TOF, Quadrupoles, Ion Traps, Orbitrap and FT-ICR
  o Ionisation techniques: EI, CI, ESI-MS, MALDI, ambient techniques
  o Fragmentation techniques and Tandem MS (small molecules and peptides)

Learning outcomes

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

- To ensure students appreciate the links between need for measurement, instrumentation design, data quality and data analysis.
- Show an advanced understanding of the: - fundamental principles behind classical analytical and spectroscopic methods. - functions of various components in complex spectroscopic instrumentation.
- Discriminate between various analytical techniques, understanding the advantages, disadvantages and current applications of each.
- Demonstrate the ability to evaluate and interpret data from a variety of measurements.
- Display practical consideration for sources and treatment of experimental error.
- Use instrumental analytical techniques in characterisation of molecules.
- Understanding of instrument construction and origin of measured signal.
- Know what signal the instrument produces and how that is transformed into the output the user receives.
- Understand how the instrument output is used to deduce molecular information.

Indicative reading list

D.A. Skoog, D.M. West, and F.J. Holler, Crouch, Fundamentals of Analytical Chemistry, 9th Edition
D.C. Harris, Quantitative Chemical Analysis, 7th edition.
Holler, Skoog, Crouch, Principles of Instrumental Analysis, 6th Edition.
Circular and linear dichroism, A. Rodger and B. Nordén, Oxford University Press, 1997
Spin Dynamics, Basics of Nuclear Magnetic Resonance, Malcolm H. Levitt, Wiley 2001, ISBN 0 471 48922 0
Primary literature in the relevant fields, to be updated annually.

View reading list on Talis Aspire

Interdisciplinary

Analytical Science is per se an interdisciplinary activity. This module is taught by experts from Analytical Chemistry, Biological Chemistry, and Physics

Subject specific skills

Subject knowledge and understanding:

- Show an advanced understanding of the:
- fundamental principles behind classical analytical and spectroscopic methods.
- functions of various components in complex spectroscopic instrumentation.
- Discriminate between various analytical techniques, understanding the advantages, disadvantages and current applications of each.
- Demonstrate the ability to evaluate and interpret data from a variety of measurements.
- Display practical consideration for sources and treatment of experimental error.
- Use instrumental analytical techniques in characterisation of molecules.
- Understanding of instrument construction and origin of measured signal.

- Know what signal the instrument produces and how that is transformed into the output the user receives.
- Understand how the instrument output is used to deduce molecular information.

Cognitive Skills:

- Critically analyse experimental data
- Comprehensively assess errors in data
- Test hypotheses using experimental data
- Interpret results with aid of information from literature.
  Subject-Specific/Professional Skills:
- Know how to prepare samples and collect data for each technique studied.
- Know how to analyse data from each technique.
- Know how to use the data to deduce molecular-level structure, dynamics and interactions.
- Understanding of instrument output versus data file produced.

Transferable skills

Understanding of team working, learning styles.
Ability to write reports, essays, papers.
Ability to present the results of research to both scientific and non-scientific audiences.
The key challenge for this module is for students to be able to understand how they operate and function in different settings and to use different skills to achieve this.

Study

Teaching split

Provider	Weighting
Chemistry	90%
Physics	10%

Study time

Type	Required
Lectures	26 sessions of 1 hour (26%)
Seminars	19 sessions of 1 hour (19%)
Other activity	3 hours (3%)
Private study	52 hours (52%)
Total	100 hours

Private study description

Self study and exam revision: 52 hours

Other activity description

Lab tours

Costs

No further costs have been identified for this module.

Assessment

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

Assessment group C6

	Weighting	Study time	Eligible for self-certification
Assessment component			
Written Reports and Presentations	50%		Yes (extension)
This will be a portfolio assignment which might include: workshop report; research literature report, laboratory visit report; research proposal “Dragon’s Den” presentation			
Reassessment component is the same			
Assessment component			
in-person examination (with computer use)	50%		No
Computer-supported, timed, in-person 2h exam; 30 min for online submission.			
Reassessment component is the same			

Feedback on assessment

Written work will be annotated and returned to students. Feedback on workshop presentation will be provided verbally.

Past exam papers for CH921

Availability

Courses

This module is Core 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 TCHA-F1PL Postgraduate Taught Molecular Analytical Science

This module is Core optional for:

- Year 1 of TMDA-B91Z Postgraduate Taught Interdisciplinary Biomedical Research

This module is Optional for:

- Year 1 of TCHA-F1PB MSc in Chemistry with Scientific Writing
- TMDA-B91Z Postgraduate Taught Interdisciplinary Biomedical Research
    - Year 1 of B91Z Interdisciplinary Biomedical Research
    - Year 1 of B91Z Interdisciplinary Biomedical Research
- Year 1 of TCHA-F1PW Postgraduate Taught Polymer Science
- TCHA-F1PE Postgraduate Taught Scientific Research and Communication
    - Year 1 of F1PE Scientific Research and Communication
    - Year 2 of F1PE Scientific Research and Communication
- Year 1 of ULFA-C1A2 Undergraduate Biochemistry (MBio)
- Year 1 of ULFA-C1A1 Undergraduate Biological Sciences (MBio)
- Year 1 of ULFA-C1A3 Undergraduate Biomedical Science (MBio)

This module is Core option list B for:

- Year 1 of TCHA-F1PY Postgraduate Taught Analytical Science and Instrumentation

This module is Option list A for:

- Year 1 of RCHA-F1P9 Postgraduate Research Analytical Science