UNIVERSITY of BRADFORD

Module Descriptor

Module Details	
Module Title	Molecular Analysis
Module Code	CFS6016-B
Academic Year	2024/5
Credits	20
School	School of Chemistry and Biosciences
FHEQ Level	FHEQ Level 6

Contact Hours	
Type	Hours
Groupwork	3
Interactive Learning Objects	11
Lectures	20
Directed Study	160
Seminars	6

Availability	
Occurrence	Location / Period
BDA	University of Bradford / Semester 1

Module Aims

This course aims to give you an advanced appreciation of the physical chemistry that underpins common analytical chemistry techniques. You will develop your skills in combining these techniques and in data analysis methods. This module will prepare you for further in-depth studies at stage-4 as well as providing a strong foundation in analytical techniques and methods for employment in analytical, materials or medicinal chemistry.

Outline Syllabus

1. Theoretical basis of NMR: vector model and energy states; origins of coupling, dipolar coupling; quantitative 1D (relaxation mechanisms); tumbling regimes and spin diffusion; two dimensional spectra principles (key components of pulse sequences).

2. Symmetry and group theory: symmetry elements and operations; assignment of point groups and character tables; reducible representations.

3. Infrared, Microwave and Raman spectroscopy: applications of symmetry; predicting vibrational spectra from symmetry elements; linear, rotational and quadratic functions in character tables.

4. Mass spectrometry: ionisation methods (electron ionisation, chemical ionisation, field ionisation; field desorption; charge transfer; fast atom bombardment; thermospray; electrospray and matrix assisted laser desorption ionisation); factors affecting fragmentation after electron ionisation mass spectrometry (ionisation and appearance energies, k versus E curves, simple cleavages versus rearrangements, primary and secondary fragment ions, the shift and even-electron rules); interpretation of electron ionisation mass spectra (particularly aromatic compounds and carbonyl compounds).

5. UV/visible and atomic absorption spectroscopy: Russell Saunders coupling; Term symbols; Microstates; Selection rules; Correlation diagrams; Beer Lambert Law.

6. Photo electron spectroscopy: Jablonski diagrams; intersystem crossing; fluorescence and phosphorescence.

7. Chromatography: HPLC, GC and GPC, Instrument set-up, columns, reverse phase and normal phase modes, plate theory, factors effecting elution time and peak shape, Langmuir and anti-Langmuir behaviour, resolution, Knox equation and Van Deemter plots, optimising experimental conditions.

8. X-ray diffraction from single crystals: unit cell determination (indexing), space group symmetry and determination from diffraction data, the phase problem and structure solution methods (Patterson and direct methods), Structure refinement and analysis. Absolute configuration determination through anomalous scattering. Crystallographic databases and data mining.

9. Case studies in combining analytical techniques to solve selected problems in inorganic and organic chemistry.

Learning Outcomes

Outcome Number	Description
01	Propose solutions to selected problems in organic and inorganic chemistry by combining information from different analytical techniques.
02	Assess the applicability of different chromatographic techniques.
03	Review the limitations of analytical data using statistical techniques.
04	Analyse the utility of spectroscopic techniques based on an appraisal of their underlying scientific principles.

Learning, Teaching and Assessment Strategy

The module uses a blended approach to support learning and achievement. Students will engage with a series of weekly online learning packages. These will include short videos that address key concepts, a set of structured activities (reading, online discussions etc.) that 'scaffold' the learning, and a range of formative tasks that generate feedback on progress. Online workshops and tutorials will also be used to support learning and monitor progress as students move through the curriculum.

You will learn how to analyse errors in your measurements, different types of data and how to choose the right data analysis techniques for different kinds of data sets and problems. We will start with mass spectrometry (MS), vibrational spectroscopies. Next, we will move onto study nuclear magnetic resonance (NMR) techniques, ultraviolet (UV)/visible and atomic absorption techniques, and X-ray diffraction.

Directed study provides you with the opportunity to undertake guided reading and to develop your own portfolio of learning to enhance transferable skills and subject knowledge. The VLE will be used to provide access to online resources, lecture notes and external links to websites of interest.

Assessment 1: An assessed proactive Team Based Learning workshop to work on given set of problems
Assessment 2: Summative examination to cover the whole module.

Mode of Assessment

Type	Method	Description	Weighting
Summative	Coursework - Written	Problem based exercise - group work (2 Hrs)	40%
Summative	Examination - Closed Book	Summative assessment - closed book exam (2 Hrs)	60%

Reading List

To access the reading list for this module, please visit https://bradford.rl.talis.com/index.html

Please note:
This module descriptor has been published in advance of the academic year to which it applies. Every effort has been made to ensure that the information is accurate at the time of publication, but minor changes may occur given the interval between publishing and commencement of teaching. Upon commencement of the module, students will receive a handbook with further detail about the module and any changes will be discussed and/or communicated at this point.
