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MODULE DESCRIPTOR

Module Title

Spectral Analysis and Interpretation

Reference	AS3070	Version	7
Created	August 2021	SCQF Level	SCQF 9
Approved	June 2002	SCQF Points	15
Amended	August 2021	ECTS Points	7.5

Aims of Module

To enable students to apply the theory of mass spectrometry, infrared, Raman, and nuclear magnetic resonance spectroscopies to the interpretation of spectra and determination of chemical structures of known and unknown compounds.

Learning Outcomes for Module

On completion of this module, students are expected to be able to:

1	Analyse IR, Raman, MS and NMR spectra in structure elucidation.
2	Use a combination of IR, Raman, MS and NMR spectra and perform data analysis from a range of advanced spectroscopic experiments.

Indicative Module Content

Use of infrared, raman, nuclear magnetic resonance spectroscopy and mass spectrometry in structure elucidation and the identification of drug molecules and other chemicals. IR and Raman Spectroscopy: The IR and Raman absorption process, sample preparation. The uses and interpretation of IR and Raman spectra. Mass Spectrometry: Theory of ionisation processes in the formation of molecular ions, mechanisms involved in base peak and other stable fragment ions, interpretation of mass spectra. NMR spectroscopy: nuclear spin states, magnetic moments, resonance absorption, continuous wave and Fourier transform instruments. 1H NMR: chemical shift, integration, spin-spin coupling, (n+1) rule, signal width and multiplicity, techniques to simplify complex spectra. 13C NMR: fully and partially decoupled spectra. An introduction to advanced techniques, DEPT, COSY, HMBC,HMQC. Combined spectral interpretation of drug molecules, paint samples and polymers in forensic and chemical applications.

Module Delivery

This is a lecture based module supplemented by tutorials and practical laboratory classes.

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Indicative Student Workload	Full Time	Part Time
Contact Hours	40	N/A
Non-Contact Hours	110	N/A
Placement/Work-Based Learning Experience [Notional] Hours	N/A	N/A
TOTAL	150	N/A
Actual Placement hours for professional, statutory or regulatory body		

ASSESSMENT PLAN

If a major/minor model is used and box is ticked, % weightings below are indicative only.

Component 1

Type:	Examination	Weighting:	70%	Outcomes Assessed:	2
Description:	Open book written examination				

Component 2

Type:	Coursework	Weighting:	30%	Outcomes Assessed:	1
Description:					

MODULE PERFORMANCE DESCRIPTOR

Explanatory Text

The first grade represents Component 1 (EX1) weighted as major and the second, Component 2 (CW1), weighted as minor. A minimum module grade of D is required for a pass, with compensation of grade E in Component 1 or Component 2 permitted. Non-submission of either component will result in an NS grade.

Module Grade	Minimum Requirements to achieve Module Grade:
A	AA, AB
B	AC, AD, AE, BA, BB, BC, CA
C	BD, BE, CB, CC, CD, DA, DB
D	CE, DC, DD, DE, EA, EB, EC
E	AF, BF, CF, DF, ED, EE, EF, FA, FB, FC, FD
F	FE, FF
NS	Non-submission of work by published deadline or non-attendance for examination

Module Requirements

Prerequisites for Module	Successful completion of Stage 2 Forensic and Analytical Science or equivalent.
Corequisites for module	None.
Precluded Modules	None.

INDICATIVE BIBLIOGRAPHY

1. PAVIA, D.L., et al. Introduction to Spectroscopy. Current Edition. 2015, 5th Edition. Harcourt
2. WATSON, D.G. Pharmaceutical Analysis a textbook for pharmacy students and pharmaceutical chemist. 2017, 4th Edition. Elsevier Edinburgh
3. SIMPSON, J. H. Organic structure determination using 2-D NMR spectroscopy: a problem-based approach. 2012 2nd Edition. Amsterdam: Elsevier
4. RAHMAN, A., CHOUDARY, M. I. AND WAHAB, A. Solving problems with NMR spectroscopy. 2016 2nd Edition. Amsterdam: Academic Press
5. LARKIN, P.J. Infrared and Raman spectroscopy: principles and spectral interpretation. 2018. 2nd Edition. Amsterdam: Elsevier