Module Title **Spectral Analysis and Interpretation** **Keywords** Infrared and raman spectroscopy, nuclear magnetic resonance spectroscopy, mass spectroscopy, spectral interpretation	Reference AS3070 SCQF SCQF Level 9 SCQF Points 15 ECTS Points 7.5 Created June 2002 Approved June 2002 Amended May 2011 Version No. 4

This Version is No Longer Current

The latest version of this module is available here

Prerequisites for Module

Basic Analytical and Spectroscopic Techniques (AS2040 and AS2041), or equivalent.

Corequisite Modules

None.

Precluded Modules

None.

Aims of Module

To enable students to apply the theory of infrared, raman, mass spectroscopy and nuclear resonance spectroscopies to the interpretation of spectra and determination of chemical structures of known and

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.

Indicative Student Workload

Contact Hours	Full Time
Lectures	20
Tutorials/Case Studies	10
Workshop	10
Directed Study	
Directed Study	63
Private Study	
Private Study	47

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 combination of IR, 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 and mass spectroscopy 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 Spectroscopy: Theory of ionisation processes in the formation of molecular ions, mechanisms involved in base peak and other stable fragment

Mode of Delivery

This is a lecture based course supplemented with tutorial sessions and workshops/case studies.

Assessment Plan

	Learning Outcomes Assessed
Component 1	2
Component 2	1

Component 1 is is a problem-solving exercise (70%)

Component 2 is a group exercise workshop (30%)

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

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 splitting, (n+1) rule, signal width and multiplicity, techniques to simplify complex spectra.

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