

Liverpool John Moores University

Title: INTERPRETATIVE SPECTROSCOPY
Status: Definitive
Code: **5002CHACAP** (113171)
Version Start Date: 01-08-2011

Owning School/Faculty: Pharmacy & Biomolecular Sciences
Teaching School/Faculty: Pharmacy & Biomolecular Sciences

Team	Leader
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Academic Level: FHEQ5 **Credit Value:** 12.00 **Total Delivered Hours:** 50.00
Total Learning Hours: 120 **Private Study:** 70

Delivery Options

Course typically offered: Semester 1

Component	Contact Hours
Lecture	36.000
Online	3.000
Practical	3.000
Workshop	6.000

Grading Basis: 40 %

Assessment Details

Category	Short Description	Description	Weighting (%)	Exam Duration
Exam	AS1	Written examination	60.0	2.00
Practice	AS2	Coursework	40.0	

Aims

To develop knowledge and practical experience of a range of spectroscopic techniques for the identification and structure elucidation of organic molecules.

Learning Outcomes

After completing the module the student should be able to:

- 1 Understand the principles and applications of a range of spectroscopic techniques.
- 2 Select an appropriate method and devise appropriate procedures for structural elucidation.
- 3 Obtain spectra from a range of different instrumentation.
- 4 Identify and determine the structure of unknown organic molecules via the interpretation of spectra.

Learning Outcomes of Assessments

The assessment item list is assessed via the learning outcomes listed:

EXAM	1	2	3	4
PRAC	1	2	3	4

Outline Syllabus

UV-Visible Spectrophotometry. Differences between atomic and molecular spectra. Electronic, rotational and vibrational contributions. Electronic transitions. Relaxation. Absorption, emission, fluorescence. Absorption spectra. Chromophores. Qualitative analysis and its limitations. Beer-Lambert law. Molar absorptivities. Calibration. Accuracy and precision. Complexation. Fieser-Woodward rules. Solvent effects. Applications. Quantitation. Analysis of mixtures by making 2 measurements. Structure elucidation. Instrumentation. Light sources., tungsten/halogen lamps, deuterium lamps. Spectrophotometers vs. photometers (monochromators vs. filters). Types of filter/monochromator. Cells. Diode array systems. Dual beam instruments. Absorption/transmission.

Infrared Spectroscopy. Absorption. Rotational and vibrational contributions. Hooke's law. Molecular symmetry/asymmetry. Stretching and bending. Diatomic, polyatomic molecules. Vibrational coupling. Factors affecting the vibrational frequency, hydrogen bonding. Basic instrumentation and sample preparation. Interpretation; fingerprint region, band assigning, functional group identification. Correlation charts and IR libraries. Applications. Structure elucidation. Support for alternative classical and spectroscopic analyses.

NMR Spectroscopy. ¹H and ¹³C NMR. Nuclear relaxation. Chemical shifts, shielding and deshielding effects, ring currents. vicinal coupling, geminal coupling. Coupling in simple aromatic systems, mono and disubstituted aromatics. Broad band ¹H decoupled ¹³C NMR, off-resonance decoupled ¹³C NMR. Sensitivity and resolution. DEPT, COSY, DQFCOSY, HETCOR, HMBC, HMQC, APT test INADEQUATE spectroscopy Fourier transformation. Gradient methods. Interpretation of data. Structure elucidation of simple organic compound.

Mass Spectrometry. Principles and applications of mass spectrometry with emphasis on practical and interpretative aspects as described in indicative

references.

In addition to traditional laboratory experiments selected to illustrate sample preparation, instrumentation and data acquisition, practical workshops will combine the use of spectroscopic methods with the interpretation of spectra in structure elucidation.

Learning Activities

Lectures, Tutorials, Workshops, Practical classes

References

Course Material	Book
Author	Pavia, D.L., Lampman, G.M., Kriz, G.S.
Publishing Year	2001
Title	Introduction to spectroscopy
Subtitle	A guide for students of organic chemistry.
Edition	3rd Edition.
Publisher	Harcourt.
ISBN	0030319617

Course Material	Book
Author	Harwood, L.M., Claridge, T.D.W.
Publishing Year	1996
Title	Introduction to organic spectroscopy.
Subtitle	
Edition	
Publisher	Oxford University Press.
ISBN	0080427987

Course Material	Book
Author	Williams, D.H., Fleming, I.
Publishing Year	1995
Title	Spectroscopic methods in organic chemistry.
Subtitle	
Edition	5th Edition.
Publisher	Mcgraw-Hill.
ISBN	0077091477

Course Material	Book
Author	Gunzler, H., Gremlich, H-U.
Publishing Year	2002
Title	IR spectroscopy
Subtitle	An introduction.

Edition	
Publisher	Wiley-VCH.
ISBN	3527288961

Course Material	Book
Author	Chapman, J.R.
Publishing Year	1996
Title	Practical organic mass spectroscopy.
Subtitle	
Edition	2nd Edition.
Publisher	Wiley.
ISBN	0471927538

Course Material	Book
Author	McLafferty, F.W., Turecek, F.
Publishing Year	1993
Title	Interpretation of mass spectra.
Subtitle	
Edition	4th Edition.
Publisher	McGraw-Hill.
ISBN	0077091477

Course Material	Book
Author	Gunther, H.
Publishing Year	1997
Title	NMR spectroscopy
Subtitle	Basic principles, concepts and applications in chemistry.
Edition	2nd Edition.
Publisher	Wiley
ISBN	047195201

Course Material	Book
Author	Claridge, T.D.W
Publishing Year	1999
Title	High resolution NMR techniques in organic chemistry.
Subtitle	
Edition	
Publisher	Elsevier Sciences
ISBN	0077091477

Course Material	Book
Author	Lambert, J. A., Shurvell, H. F., Lightner, D. A., Cooks, G.G.
Publishing Year	1998
Title	Organic Structural Spectroscopy
Subtitle	
Edition	
Publisher	Prentice-Hall

ISBN	0132586908
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Course Material	Book
Author	Smith, R.M.
Publishing Year	2004
Title	Understanding Mass Spectra: A Basic Approach
Subtitle	
Edition	2nd
Publisher	John Wiley & Sons
ISBN	047142949X

Course Material	Book
Author	de Hoffmann, E., Stroobant, V.
Publishing Year	2001
Title	Mass Spectrometry: Principles and Applications
Subtitle	
Edition	2nd
Publisher	John Wiley & Sons
ISBN	0471485667

Course Material	Book
Author	Gross, J.H.
Publishing Year	2004
Title	Mass Spectrometry: A Textbook.
Subtitle	
Edition	
Publisher	Springer Verlag
ISBN	3540407391

Course Material	Book
Author	Lee, T.A.
Publishing Year	1998
Title	A Beginner's Guide to Mass Spectral Interpretation.
Subtitle	
Edition	
Publisher	John Wiley & Sons
ISBN	0471976296

Notes

This module is designed to provide students with a knowledge of the theory and application of spectroscopic methods of analysis. An in depth study and comparison of several different spectroscopic methods applied to the elucidation of molecular structures is carried out. The lectures are supported with practical experience of the spectroscopic techniques and workshops on the interpretation of classical data and spectra in the determination of the structure of unknown compounds.

