ZCHE C3104: Spectrochemical Methods

Module Title:	Spectrochemical Methods
Language of Instruction:	English

Credits:	10

NFQ Level:	7

Module Delivered In	2 programme(s)

Teaching & Learning Strategies:	This module will be taught as four 1-hour lectures per week and 16 x 3-hour laboratory practical sessions delivered on a rota. The instruction will be a mix of traditional lecturing and student-centered learning. Theory and practical module content will be synchronised and questions relating to the material will be discussed during the theory class and/or during practical sessions. There is a possibility that some of the CA or practical work will be done in collaboration when an international partner. Analytical websites will be incorporated during independent study.

Module Aim:	This module further develops the theory and practice of analytical chemistry, with specific reference to the areas of atomic and molecular spectroscopy.

Learning Outcomes	
On successful completion of this module the learner should be able to:	
LO1	Describe background chemistry and theory of the principal types of spectroscopy.
LO2	Demonstrate with confidence a wide variety of spectrochemical applications.
LO3	Apply the theoretical principles of atomic and molecular spectroscopy to industrial, pharmaceutical and environmental analysis.
LO4	Employ the development and execution of laboratory assays, according to best practice

Pre-requisite learning
Module Recommendations *This is prior learning (or a practical skill) that is recommended before enrolment in this module.*
No recommendations listed
Incompatible Modules *These are modules which have learning outcomes that are too similar to the learning outcomes of this module.*
No incompatible modules listed
Co-requisite Modules
No Co-requisite modules listed
Requirements *This is prior learning (or a practical skill) that is mandatory before enrolment in this module is allowed.*
Successful completion of year 2 or equivalent

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Module Content & Assessment

Indicative Content
Fundamentals A review of: Interaction of electromagnetic radiation with matter. Absorption, emission. Beer's Law. Evaluation and interpretation of analytical data, standard operating procedures (SOP), calibration.
Sample pre-treatment Wet digestion, microwave digestion, and ashing. Safety considerations, estimations. Interferences.
Atomic spectroscopy A review of electronic transitions. Selection rules for absorption and emission of energy. Flame, non-flame, and electrical methods of atomisation (Graphite furnace, inductively coupled plasma (ICP), vapour method (Hg), hydride (Se,As)). Understanding of interferences due to flame, matrix, and sample components, and compensation for and elimination of interferences will be strengthened through practical work.
Molecular spectroscopy Understanding of deviations from Beer's Law, solvents, cells, chromophores, electronic transitions ($\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$), molar absorptivity (ε) values, effect of conjugation on absorption will be strengthened. Ligand-field, crystal-field and charge-transfer theories. Use of single/multiple standards, multi-component, derivatives. Fluorescence and phosphorescence.
Infrared spectroscopy Vibrational and rotational transitions.Mid-Infrared, Near Infrared (NIR). Rotor and spring models for spectra of diatomic (HCl) and polyatomic species. 3N-5, 3N-6 formulae, allowed/ forbidden transitions. Identification of compounds using correlation charts, spectral libraries. ATR (attenuated total reflectance). Fourier Transform IR, solvents effects, adjacent groups. Applications: gas monitoring, aqueous solutions, coatings, films.
Nuclear Magnetic Resonance Spectroscopy Nuclear spin states and magnetic moments, resonance, relaxation, chemical shift, factors affecting chemical shift, shielding. FT spectrometers, FID. First order spectra, spin-spin coupling, multiplicity, chemical equivalence, relationship between spectra and structure for 1H NMR. Outline of 13C NMR, 2D techniques, and multinuclear NMR.
Related matters Applications to synthetic, kinetic and mechanistic studies. Outline of mass spectroscopy, x-ray fluorescence; hyphenated GC-MS and ICP-MS. Overview of related environmental, medical, biological methods and art conservation. Assay method development. Luminescence in forensic analysis. Fingerprints and identification of bodily fluids.
Practical Practical work will proceed in parallel with theoretical concepts, building on previous experience. Students will perform practical work to explore sample preparation and resolution of interference effects in Atomic Absorption and Flame Photometry. A systematic approach to uv-visible spectrometric methods will elucidate colour and complex formation; students will learn to determine single and multi-component analytes. Gas, liquid and solid phase sampling methods will be followed by FTIR spectroscopy.

Assessment Breakdown	%
Continuous Assessment	30.00%
Practical	40.00%
End of Module Formal Examination	30.00%

Special Regulation
Students must achieve a minimum grade (35%) in both the practical/CA and final examination

Continuous Assessment

Assessment Type	*Assessment Description*	*Outcome addressed*	*% of total*	*Assessment Date*
Case Studies	Two continuous assessments throughout year. When possible, one of these will include collaboration with an international partner.	1,2,3	30.00	n/a

No Project

Practical

Assessment Type	*Assessment Description*	*Outcome addressed*	*% of total*	*Assessment Date*
Practical/Skills Evaluation	Worksheets and reports; Practical Log Book	3,4	40.00	n/a

End of Module Formal Examination

Assessment Type	*Assessment Description*	*Outcome addressed*	*% of total*	*Assessment Date*
Formal Exam	3 hour exam	1,2,3	30.00	End-of-Semester

SETU Carlow Campus reserves the right to alter the nature and timings of assessment

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Module Workload

Workload: Full Time		
Workload Type	*Frequency*	*Average Weekly Learner Workload*
Lecture	12 Weeks per Stage	4.00
Laboratory	12 Weeks per Stage	4.00
Estimated Learner Hours	15 Weeks per Stage	10.27
	Total Hours	250.00

Module Delivered In

Programme Code	Programme	Semester	Delivery
CW_SAPHA_B	Bachelor of Science (Honours) in Pharmaceutics and Drug Formulation	5	Mandatory
CW_SAASC_D	Bachelor of Science in Analytical Science	5	Mandatory