Title:	Structure Elucidation & BioMol APPROVED
Long Title:	Structure Elucidation & Bioactive Mol.

Module Code:	CHEA9003	**Duration:**	1 Semester

Credits:	10
NFQ Level:	Expert
Field of Study:	Analytical Chemistry
Valid From:	Semester 1 - 2021/22 (September 2021)
Module Delivered in	2 programme(s)
Module Coordinator:	Donagh OMahony
Module Author:	Eileen OLeary
Module Description:	This module introduces the student to the chemical structure of organic and bioactive molecules and links structural features with appropriate analytical techniques to facilitate structural elucidation. It introduces students to organic chemistry reactions and mechanisms and their importance in predicting side products and degradation products leading to impurities in processes. It challenges students to engage in the process approach and find suitable methods or approaches to prevent, detect, separate and quantify impurities and produce pure products.

Learning Outcomes	
On successful completion of this module the learner will be able to:	
LO1	Model and identify the functional groups and structural features of organic and bioactive molecules.
LO2	Determine the products of fundamental chemical reactions, predict potential impurities and discuss the importance of understanding chemical reactions in the process of developing detection and quantitation methods.
LO3	Generalize molecular structures as acidic or basic, estimate pKa values and recommend modifications to extraction and purification methods based on scientific logic.
LO4	Generalize molecular structures as acid or base sensitive, anticipate degradation products.
LO5	Propose and evaluate analytical techniques appropriate to analysing organic and bioactive molecules, comparing the methods and indicating their limitations.
LO6	Analyse, interpret and compare spectral data for a variety of organic and bioactive molecules to justify and support decision making.
LO7	Lead discussion in relation to choice of analytical techniques, specific to detection, identification and quantitation of organic and bioactive molecules.

Pre-requisite learning
Module Recommendations *This is prior learning (or a practical skill) that is strongly recommended before enrolment in this module. You may enrol in this module if you have not acquired the recommended learning but you will have considerable difficulty in passing (i.e. achieving the learning outcomes of) the module. While the prior learning is expressed as named CIT module(s) it also allows for learning (in another module or modules) which is equivalent to the learning specified in the named module(s).*
Incompatible Modules *These are modules which have learning outcomes that are too similar to the learning outcomes of this module. You may not earn additional credit for the same learning and therefore you may not enrol in this module if you have successfully completed any modules in the incompatible list.*
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. You may not enrol on this module if you have not acquired the learning specified in this section.*
No requirements listed

Module Content & Assessment

Indicative Content
Chemical Structure and Representations Functional groups, structural representations, structural isomers, stereoisomers, polarity (solvent and molecule), bonding, molecular formula, degree of unsaturation, conjugation.
Acidity and basicity Acidity, basicity, pKa values, acid sensitive functional groups, base sensitive functional groups, buffers, degradation products, liquid-liquid extraction.
Reactions & Mechanisms Organic reactions, oxidation, reduction, elimination, substitution, hydrolysis, derivatization reactions, impurity/side product formation, degradation products.
Analytical Methods and Chemical Structure Elucidation NMR (proton and carbon), Mass spectrometry, Infrared spectroscopy, UV Spectroscopy, Thin layer Chromatography, HPLC, UPLC, GC.
Problem Solving Analysis, interpretation and correlation of spectral data for organic and bioactive molecules. Predict impurities, side products, degradation products and appropriate methods for their detection and quantitation.

Assessment Breakdown	%
Course Work	100.00%

Course Work

Assessment Type	*Assessment Description*	*Outcome addressed*	*% of total*	*Assessment Date*
Project	Engage in pairs in the sourcing, investigation and design of Authentic Problems and outline and share solutions with peers.	1,2,3,4,5,6,7	20.0	Every Second Week
Project	Team Project: Propose, evaluate and present on appropriate analytical methods suitable for separating, detecting, identifying and quantifying specific organic and bioactive molecules including formation of side products and degradation products.	2,3,4,5,6,7	30.0	Week 12
Short Answer Questions	On-line knowledge check quizzes, comprising a variety of questions styles.	1,2,3,4,5,6,7	20.0	Every Second Week
Oral Examination/Interview	Oral Exam: Scenario Based Assessment, Engage in an oral examination which mimics an interview for a role in Analytical Science and Method Validation	1,2,3,4,5,6,7	30.0	Week 13

No End of Module Formal Examination

Reassessment Requirement
Coursework Only *This module is reassessed solely on the basis of re-submitted coursework. There is no repeat written examination.*

The institute reserves the right to alter the nature and timings of assessment

Module Workload

Workload: Full Time				
Workload Type	*Workload Description*	*Hours*	*Frequency*	*Average Weekly Learner Workload*
Tutorial	Interactive workshop and problem solving sessions	2.0	Every Week	2.00
Lecture	Theory and in-class engagement in problem solving and applying learning	2.0	Every Week	2.00
Independent & Directed Learning (Non-contact)	Personal Study and Assignment Preparation	10.0	Every Week	10.00
			Total Hours	14.00
			Total Weekly Learner Workload	14.00
			Total Weekly Contact Hours	4.00

Workload: Part Time				
Workload Type	*Workload Description*	*Hours*	*Frequency*	*Average Weekly Learner Workload*
Tutorial	Interactive workshop and problem solving sessions	2.0	Every Week	2.00
Lecture	Theory and in-class engagement in problem solving and applying learning	2.0	Every Week	2.00
Independent & Directed Learning (Non-contact)	Personal Study and Assignment Preparation	10.0	Every Week	10.00
			Total Hours	14.00
			Total Weekly Learner Workload	14.00
			Total Weekly Contact Hours	4.00

Module Resources

Recommended Book Resources

- **Robert J. Ouellette and J. David Rawn 2015, *Principles of Organic Chemistry (https://ebookcentral.proquest.com/lib/cit-ebooks/detail.action?docID=1962520)***
- **Robert J. Ouellette and J. David Rawn 2014, *Organic Chemistry : Structure, Mechanism, and Synthesis (https://ebookcentral.proquest.com/lib/cit-ebooks/detail.action?docID=1710540)***
- **Yong-Cheng Ning, John Wiley and Sons Ltd 2005, *Structural identification of organic compounds with spectroscopic techniques* [ISBN: 3527312404]**
- **Timothy D. W. Claridge, Elsevier Science & Technology, https://ebookcentral.proquest.com/lib/cit-ebooks/detail.action?docID=4513900 2016, *High-Resolution NMR Techniques in Organic Chemistry***
- **Maria-Magdalena Cid, Jorge Bravo, and Jorge Bravo, John Wiley & Sons, Incorporated, https://ebookcentral.proquest.com/lib/cit-ebooks/detail.action?docID=1911672 2015, *Structure Elucidation in Organic Chemistry : The Search for the Right Tools***

Supplementary Book Resources

- **Andrew B. Hughes 2015, *Amino Acids, Peptides and Proteins in Organic Chemistry, Analysis and Function of Amino Acids and Peptides (https://ebookcentral.proquest.com/lib/cit-ebooks/detail.action?docID=1129766)***
- **Rensheng Xu, Yang Ye, and Weimin Zhao, *Introduction to Natural Products Chemistry (https://ebookcentral.proquest.com/lib/cit-ebooks/detail.action?docID=1446287)***
- **Jan-Christer Janson and Jan-Christer Janson (https://ebookcentral.proquest.com/lib/cit-ebooks/detail.action?docID=675104) 2011, *Protein Purification : Principles, High Resolution Methods, and Applications (***
- **Vladimir Havlicek and Jaroslav Spizek, *Natural Products Analysis : Instrumentation, Methods, and Applications (https://ebookcentral.proquest.com/lib/cit-ebooks/detail.action?docID=1789984)***

This module does not have any article/paper resources

This module does not have any other resources

Module Delivered in

Programme Code	Programme	Semester	Delivery
CR_SASIV_9	MSc in Analytical Sciences with Instrument Validation	2	Mandatory
CR_SANIV_9	Postgraduate Diploma in Analytical Sciences with Instrument Validation	2	Mandatory