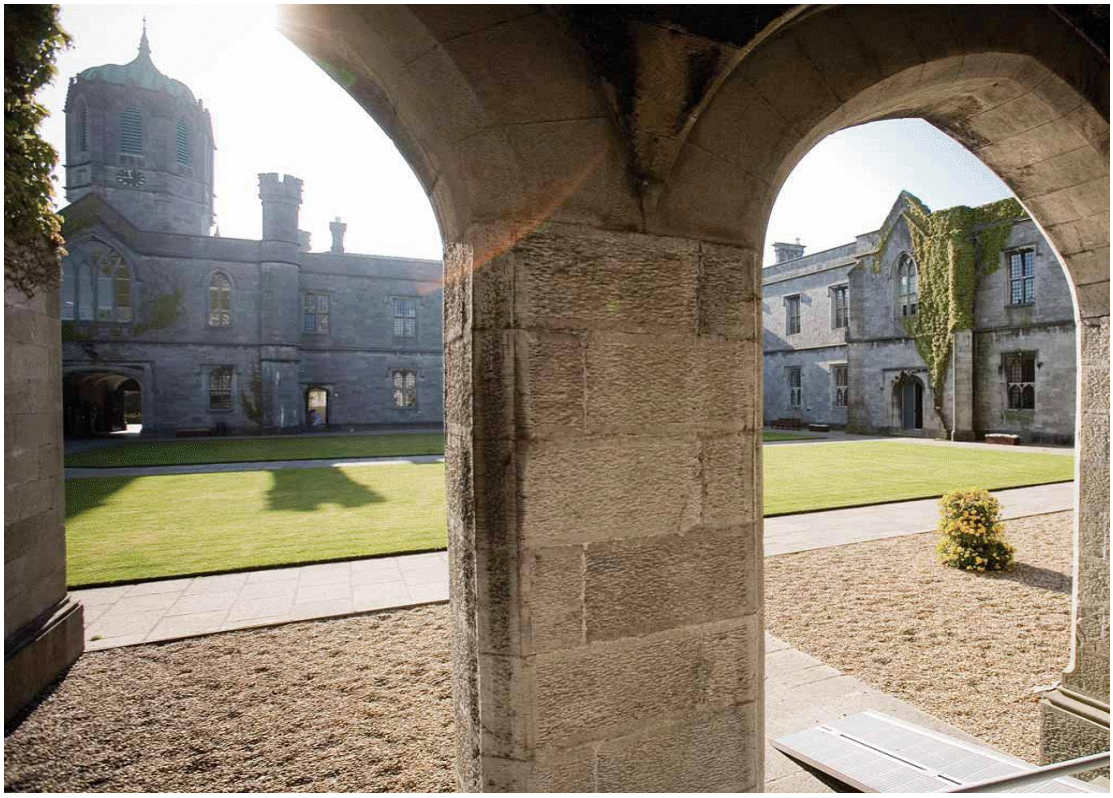
NUI Galway
OÉ Gaillimh

SCHOOL OF BIOLOGICAL AND CHEMICAL SCIENCES



4th Year Chemistry

Information Booklet

2022-2023

CONTENTS

***subject to change**

SUMMARY OF COURSE STRUCTURE 2022-2023

Semester I

	Examination
Research Investigation (CH4101, 20 ECTS)	continuous assessment
Analytical chemistry (CH448, 5 ECTS)	continuous assessment (4 tests)
Practical Skills Development (CH451, 5 ECTS)	continuous assessment

Semester II

Physical Chemistry (CH429, 5 ECTS)	2 h Exam paper + 2 CA
Biophysical Chemistry (CH432, 5 ECTS)	2 h Exam paper + 2 CA
Bioinorganic Chemistry (CH438, 5 ECTS)	2 h Exam paper + 2 CA
Advanced Inorganic Chemistry (CH445, 5 ECTS)	2 h Exam paper + 2 CA
Bioinorganic and Inorganic Medicinal Chemistry (CH446, 5 ECTS)	2 h Exam paper + 2 CA
Organic Chemistry (CH4113, 5 ECTS)	2 h Exam paper + 2 CA

Notes on workload expected for each module

Workload for a 5 Credit Module **125 h**

The workload includes the teaching contact with staff & autonomous learning.
Autonomous learning & working includes time spent working independently carrying out assignments, learning, revising, additional reading. Normally this is 4 times that of the contact time spent with staff. Thus the contact time with staff in each module above is 25 h and students would be expected to spend over 100 h working independently studying these modules.

Continuous assessment in Semester II

The continuous assessment will be in the form of in-class tests during the teaching semester that will be graded. The 2 CA will contribute 20% of the overall grade for each module.

SEMESTER I AND II TIMETABLES

SEMESTER I

Week Beginning	5-Sep	12-Sep	19-Sep	26-Sep	3-Oct	10-Oct	17-Oct	24-Oct	31-Oct	7-Nov	14-Nov	21-Nov	28-Nov	5-Dec	12-Dec
Spectroscopic and Physical Methods and Application - CH448															
Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Mon 10-11 , Room 231	OT	LR	OT	LR	OT	LR	OT	LR	**Bank Holiday**						
Mon 11-12 , Room 231	OT	LR	OT	LR	OT	LR	OT	LR							
Thu 10-11 , Room 231	OT	LR	OT CA	LR CA	OT	LR	OT CA	LR CA							
Practical Skills Development - CH451															
Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Tues 10-11, Room 231	PC	PC	PC						**Bank Holiday**						
Research Investigation - CH4101															
Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Mon	2-4pm Safety	Research (Mon-Fri; 25-35 h per week)			Research	Research (Mon-Fri; 25-35 h per week)					Research	Write-up		Project Submission deadline ***Thursday 8th December at 15.00***	Presentation on Project to be held this week
Tue	Research														
Wed	Research				***Meeting with 2nd Reader***						***eting with 2nd Read***				
Thu	Research														
Fri	2-4pm **Induction**				Research						Research				

SEMESTER II

Week Beginning	9-Jan	16-Jan	23-Jan	30-Jan	6-Feb	13-Feb	20-Feb	27-Feb	6-Mar	13-Mar	20-Mar	27-Mar	10-Apr	17-Apr/5-May
Bioinorganic and Inorganic Medicinal Chemistry - CH446													STUDY WEEK	Exams
Week	1	2	3	4	5	6	7	8	9	10	11	12		
Mon 10-11, Dillon	Metals in Medicine (AE)				Bank Holiday	Metalloproteins (AE)		Biomineralization(SVE)			Tutorial (AE)	Tutorial (SVE)		
Wed 4-5, Larmor					Test						Tutorial (AE)			
Wed 5-6, Larmor											Tutorial (AE)			
Physical Chemistry - CH429														
Week	1	2	3	4	5	6	7	8	9	10	11	12		
Mon 9-10, AC202	HC	HC	HC	HC	Bank Holiday	CZ	CZ	CZ	CZ		HC	CZ		
Tues 4-5, Larmor	HC	HC	HC	HC		CZ	CZ	CZ	CZ		HC	CZ		
Tues 5-6, Larmor	HC	HC	HC	HC	Test	CZ	CZ	CZ	CZ		HC	CZ		
Biohysical Chemistry - CH432														
Week	1	2	3	4	5	6	7	8	9	10	11	12		
Tues 9-10, AC202	DC	DC	DC	DC		ML	ML	ML	ML					
Tues 10-11, AC202	DC	DC	DC	DC		ML	ML	ML	ML					
Thu 1-2, Dillon	DC	DC	DC	DC		ML	ML	ML	ML					
Bioorganic Chemistry -CH438														
Week	1	2	3	4	5	6	7	8	9	10	11	12		
Mon 3-4, Larmor	PC	PC	PC	PC	Bank Holiday	SvE	SvE	SvE	SvE					
Mon 4-5, Larmor	PC	PC	PC	PC	Bank Holiday	SvE	SvE	SvE	SvE					
Thu 10-11, AC202	PC	PC	PC	PC	Test	SvE	SvE	SvE	SvE					
Organic Chemistry - CH4113														
Week	1	2	3	4	5	6	7	8	9	10	11	12		
Tue 12-1, Dillon	EM	EM	EM	EM		PM	PM	PM	PM	Test	EM	PM		
Fri 2-3, Kirwan	EM	EM	EM	EM	Test	PM	PM	PM	PM	**Bank Holiday**	EM	PM		
Fri 3-4, Kirwan	EM	EM	EM	EM		PM	PM	PM	PM	**Bank Holiday**	EM	PM		
Advanced Inorganic Chemistry - CH445														
Week	1	2	3	4	5	6	7	8	9	10	11	12		
Thurs 2-3, Dillon	CP	CP	CP	CP	Test	PF	PF	PF	PF	Test	CP	PF		
Fri 10-11, AC202	CP	CP	CP	CP		PF	PF	PF	PF	**Bank Holiday**	CP	PF		
Fri 11-12, AC202	CP	CP	CP	CP		PF	PF	PF	PF	**Bank Holiday**	CP	PF		

CH448: SPECTROSCOPIC AND PHYSICAL METHODS AND APPLICATIONS (SEMESTER I)

Staff: Prof. Olivier Thomas (coordinator), Dr. Luca Ronconi

The main objectives of this module are to provide the necessary background in analytical chemistry to perform the 4th year project in the best conditions. No final exam will be organised and the assessment will be performed through two tests in each of the following parts

1. NMR and mass spectrometry for organic molecules (12 h)
2. Analytical techniques for inorganic molecules (12 h)

Course Topics:	Learning Outcomes
PART 1: Organic molecules (12 h including 2 h of test)	
1D NMR experiments including ^{1}H, ^{13}C DEPT Other nuclei	Understand the basics of 1D NMR experiments. How to perform an experiment. How to interpret data of a 1D NMR experiment. Number of qC, CH, CH_2 and CH_3. Applications to other nuclei such as F and P.
2D NMR experiments to establish the planar structures of organic molecules	Be able to use COSY experiments to build Spin Coupled Systems. Be able to use HSQC/HMQC experiments to complete the SCS. Link the different SCS and heteroatoms using HMBC spectra.
Coupling constant values interpretation for cyclic compounds and couble bonds Spatial coupling such as ROESY and NOESY experiments to gain insights into the 3D structures of (bio)organic molecules	Be able to use nOe and coupling constant values to propose relative configurations of organic molecules.
Mosher method	Use Mosher method to assess the absolute configuration of organic molecules
Mass spectrometry low and high resolution	Use data from low and mass spectrometry to obtain information such as the molecular formula of organic molecules. Use of chemcalc
Structure elucidation of organic molecules	Understand how to elucidate the 2D and then 3D structures of organic molecules using NMR and MS data.
PART 2: Inorganic molecules (12 h including 2 h of test)	
Electronic spectra of metal complexes (microstates, spectroscopic terms, Russell-Saunders coupling, spin-orbit coupling, Racah parameters, Tanabe-Tsugano diagrams);	Understand and use of the electronic transitions of metal complexes
IR spectroscopy of transition metal complexes (focusing on metal–other atoms vibrations in the far IR region);	Understand the data obtained for IR spectra of inorganic molecules
Solution NMR spectroscopy of transition metal complexes (focusing on the direct detection of NMR-active nuclei other than 1H, 13C, 15N and 31P);	Use of spectroscopic techniques to derive the structure and to understand the properties of transition metal complexes.

CH451: PRACTICAL SKILLS DEVELOPMENT (SEMESTER I)

Staff: Prof. Peter Crowley (coordinator), Dr Eddie Myers

The purpose of this 5 credit module is for you to become familiar with key aspects of research and to prepare you for CH4101. You will complete CH451 within the first 3 weeks of semester I. The module has six components (Table 1) including a mini-report that you submit to your project supervisor before **4 pm on Friday 23 September 2022**.

Table 1. CH451 module components

#	Component*	Task
1	Induction (<1 page)	Learn about your host laboratory. What is the main aim of the laboratory and what are your roles both in research and in contribution to the laboratory.
2	Health & Safety (>2 pages)	Health and safety is paramount to research. Attend the H&S briefing, prepare your project risk assessment (PRA) and a standard operating procedure (SOP) – see details below.
3	Summary and literature search (2 pages)	Use Scopus to find relevant literature. Demonstrate the funnel approach, from identifying the broad topic to distinguishing specific papers. Write a short summary including project aim (one sentence); project objectives (three bullet points); how your project will contribute to state of the art (one paragraph); methods / approach you will use to address the project (one paragraph); a self-made graphic that captures the essence of your project; a project timeline and at least 6 references.
4	Practical skills (1 page)	Identify a technique that is central to your project. Get training in that technique and document the main steps required. Include representative data, that you obtained and explain the uses/limitations of the technique.
5	Experiment design (<1 page)	Scientific research is about (dis)proving hypotheses. When correctly performed, experiments can be used to test a hypothesis. A properly designed experiment includes controls. Describe an example of good experiment design for your project.
6	Mini-report	Document your completion of components 1 – 5 with PRA, SOP and other supporting documentation appended.

*Indicative page count in the mini-report.

Health and Safety

Health and safety is essential when designing and performing experiments, and handling, analysing, storing or disposing of chemicals. You should strive to be aware of all possible ways your work could adversely affect you, your colleagues and the environment. Take steps to prevent or mitigate that impact.

You will be assessed on the following:

A. Participation in the Health and Safety Briefing at 2-4 pm, Monday 5th September 2022.

B. Preparation of a project risk assessment by using the template provided and in consultation with your supervisor. The completed form is signed by you and your supervisor and sent to the Health and Safety Officer (Dr. Myers) before experiments begin.

C. Preparation of a standard operating procedure (SOP) for the use of a chemical or the performance of a technique that is relevant to your project. This SOP will be added to the School's health and safety documentation, which will be available to other researchers.

D. Identification and documentation of the health and safety risks of each experiment before the experiment is performed. This documentation will be made available to your second assessor during scheduled meetings or be presented to the School's Health and Safety Officer upon request during lab audits.

General Health and Safety Rules

- Never work alone
- Laboratory work is within core hours, 9 am – 6 pm.
- Protective clothing, safety glasses and coat, must be worn in the laboratory
- No food or drink is permitted in the laboratory
- Headphones/earbuds are not permitted in the laboratory

Failure to adhere to the general rules will lead to disciplinary action. Repeated and/or blatant disregard for health and safety will result in dismissal from the research laboratory.

Project Risk Assessment

General Information

Researcher Name	Click or tap here to enter text.
Student/Staff ID	Click or tap here to enter text.
Researcher Type	Undergraduate Student
Research Group	Click or tap here to enter text.
Research Location	Click or tap here to enter text.
	Room risk assessment available: ☐Yes ☐No See Note 1 Room risk assessment read: ☐Yes ☐No
Start of Research Period	Click or tap to enter a date.
End of Research Period	Click or tap to enter a date.
Project Title	Click or tap here to enter text.
Project Description	Outline main aims, objectives, methods and materials. Can be written in general form to avoid revealing sensitive or confidential information

Chemicals/biological agents/materials you will be using in the laboratory

Material Type	Some materials can be banded (for example, cyclohexanes, ethyl acetate, toluene). Materials with special hazards should be addressed separately (e.g. carcinogenic materials, such as dichloromethane or dimethylformamide).
Material Hazards and Mitigation Measures	Describe the main hazards and list the appropriate H codes associated with the material. Outline measures that are in place in your laboratory or the precautions you will be taking to mitigate these hazards.
	SDS available locally: ☐Yes ☐No See Note 2 SOP available: ☐Yes ☐No Risk assessment available: ☐Yes ☐No

To add information for another material, click on the table above and then click on the '+' sign on the bottom right

Techniques you will be using in the laboratory:

Description of technique	for example – Liquid-liquid extraction by using a separating funnel
Technique Hazards and Mitigation Measures	What are the main hazards in terms of your specific use of this technique. What mitigation measures will you be taking
	SOP available: ☐Yes ☐No See Note 3

To add information for another technique, click on the table above and then click on the '+' sign on the bottom right

Equipment you will be using in the laboratory

Equipment Type	General name/description; for example – Rotary Evaporator with single-pass water condenser and diaphragm vacuum pump
Equipment Hazards and Mitigation Measures	What are the main hazards in terms of your specific use of the equipment. What mitigation measures will you be taking
	SOP available: ☐Yes ☐No See Note 4 Risk assessment available: ☐Yes ☐No

To add information for another piece of equipment, click on the table above and then click on the '+' sign on the bottom right

Training:

Safety Briefing	Have you attended a local safety briefing? ☐Yes ☐No When did this event take place? Click or tap to enter a date.
Fire Safety	Have you attended a formal fire safety event? ☐Yes ☐No When did this event take place? Click or tap to enter a date.

	Are you a trained fire marshal? ☐Yes ☐No When were you trained? Click or tap to enter a date. Have you been given informal fire safety training and information specific to your work area? ☐Yes ☐No Who provided this training? Name Have you taken part in a fire drill here? ☐Yes ☐No When did the most recent drill take place? Click or tap to enter a date. Where is the closest fire alarm call point? Enter location here Where is the closest set of fire extinguishers? Enter location here Where is your fire assembly point? Letter.
First aid	Are you a trained first aider? ☐Yes ☐No When were you trained? Click or tap to enter a date. Name three first aiders available in your area. Name of First Aider 1 Name of First Aider 2 Name of First Aider 3. Where is your closest first aid kit? Enter location here Where is the closest eye-wash station? Enter location here Where is the closest emergency shower? Enter location here

Training Courses Available (See Note 5)

Manual Handling Required? ☐Yes ☐No Completed? Click or tap to enter a date.

Ergonomics & Light Manual Handling Required? ☐Yes ☐No Completed? Click or tap to enter a date.

Compressed Gas Required? ☐Yes ☐No Completed? Click or tap to enter a date.

Risk Assessments (BB) Required? ☐Yes ☐No Completed? Click or tap to enter a date.

Basic Principles for the Safe Use of Chemicals (BB) Required? ☐Yes ☐No Completed? Click or tap to enter a date.

Laboratory Safety Management (BB) Required? ☐Yes ☐No Completed? Click or tap to enter a date.

Chemical Banding (BB) Required? ☐Yes ☐No Completed? Click or tap to enter a date.

Nanomaterials Risk Assessment (BB) Required? ☐Yes ☐No Completed? Click or tap to enter a date.

Fieldwork Risk Assessment (BB) Required? ☐Yes ☐No Completed? Click or tap to enter a date.

Other Identified Training Needs (See Note 6)	
Enter Training Type	Completed? Click or tap to enter a date.
Enter Training Type	Completed? Click or tap to enter a date.
Enter Training Type	Completed? Click or tap to enter a date.

Additional Expectations

(a) In addition to this project risk assessment, you are required to perform an individual risk assessment for every experiment. This risk assessment should be documented in a form, which should be stored in an appropriate folder within your research group's Teams/Sharepoint site, or in your laboratory notebook.

(b) Undergraduate researchers are only allowed to work in the laboratory during core working hours (Monday – Friday, 9:00 – 18:00). For all other researchers, laboratory work can be conducted outside of working hours, but only when other researchers are present. High-risk experiments should only be conducted during core hours.

(c) In the event of an accident or a near miss, both your supervisor and a member of the Health & Safety Committee should be informed as soon as is practicable. An accident/near-miss report form will need to be completed within 24 hours and sent to the Health and Safety Committee, who will forward it to the Head of School and the University Health & Safety Office (https://www.nuigalway.ie/health-safety/accident-reporting/). You will also be asked to engage with a School investigation to ensure that measures are put in place to avoid such adverse events in the future.

I have read and understood the points above ☐

Signature of Researcher	**Date**
	Click or tap to enter a date.
Signature of Principal Investigator	**Date**
	Click or tap to enter a date.

Notes:

1 If a room risk assessment is not available, inform your supervisor/principal investigator, who will organize for a risk assessment to be prepared. If you are working in several areas/rooms/laboratories, a risk assessment is required for each one.

2 An up-to-date SDS will need to be stored in an appropriate folder in your research group's Teams/Sharepoint site. Banded risk assessments are available on the School's Health and Safety Sharepoint site. Particularly hazardous materials (e.g. CMRs) will need a separate SOP/risk assessment. If appropriate SOPs/risk assessments are not available, it is the responsibility of your PI to ensure that one is prepared. New SOPs/risk assessments should be sent to the School's Health and Safety Committee for approval and upload to the School's Health and Safety Sharepoint site.

3 If appropriate SOPs/risk assessments are not available, it is the responsibility of your PI to ensure that one is prepared. New SOPs/risk assessments should be sent to the School's Health and Safety Committee for approval and upload to the School's Health and Safety Sharepoint site.

4 Your research group should have a list of available pieces of equipment. Each piece of equipment should have an SOP and a risk assessment. If appropriate SOPs/risk assessments are not available, it is the responsibility of your PI to ensure that one is prepared. New SOPs/risk assessments should be sent to the School's Health and Safety Committee for approval and upload to the School's Health and Safety Sharepoint site.

5 Please refer to the University's Safety Training site for information on available training courses. Some courses are available on Blackboard (BB).

6 If a particular type of training appears to be unavailable, please note the training need in this form and contact the School's Health and Safety Committee, who may be able to organize such training centrally at the University/College/School level. However, in some cases, this training will need to be organized by your PI.

CH429: PHYSICAL CHEMISTRY (SEMESTER II)

Staff: Prof. Henry Curran (coordinator), Dr Chongwen Zhou

1. Chemical Kinetics
2. Statistical Thermodynamics
3. Quantum Mechanics

1. Chemical Kinetics

Students will be able to:

- Derive the rate law for a first and second order reaction and from that determine the half-life for a reaction and the rate of reaction.
- Determine the kinetics for an elementary reaction.
- Explain the kinetics associated with flow reactors, jet-stirred reactors and shock tubes.
- Understand how the rate constant of a reaction varies with temperature and derive the frequency A-factor and activation energy of a reaction given the rate constant and different temperatures.
- Appreciate and understand the dependence of kinetics on thermodynamics of reactants and products.
- Understand Photochemical Kinetics and its application to real world problems.
    - Understand Photolytic activation and flash photolysis
    - Understand fast reactions and how these can be studied
- Theories of reaction rates
    - Understand and apply Simple Collision Theory

2. Statistical Thermodynamics

- Know that the Boltzmann distribution that gives the number of molecules in each state of a system at any temperature is given by the equation: $N_i = Ne^{-E_i/kT}/q$
- The partition function is defined as: $q = \sum_i e^{-E_i/kT}$ and is an indication of the number of thermally accessible states at the temperature of interest.
- The molecular partition function is the product of the contribution from translation, rotation, vibration, electronic and spin distributions: $q = q^T q^R q^V q^E q^S$
- The translational partition function is: $q^T = (2\pi mkT)^{3/2}V/h^3$
- The vibrational partition function is: $q^V = 1/(1-e^{-h\omega/kT})$
- The rotational partition function is: $q^R = kT/\sigma hB$, where $\sigma = 1$ for an unsymmetrical linear rotor and $\sigma = 2$ for a symmetrical linear rotor.
- The electronic partition function is: $q^E = 1$ for closed-shell molecules with high-energy excited states.
- The internal energy is: $U = U(0) + E$, with $E = (NkT^2/q) \times$ slope of q plotted against T.
- The Boltzmann formula for the entropy is $S = k \ln W$, where W is the number of different ways in which the molecules of a system can be arranged while keeping the same total energy.
- The standard molar Gibbs energy is $G_m^\circ - G_m^\circ(0) = -RT\ln(q_m^\circ / N_A)$

3. Quantum Mechanics

Students will gain an appreciation of

- fundamentals of quantum mechanics - quantization, uncertainty principle, the Schrodinger equation and its application to particle in a box and the rigid rotator
- the hydrogen(ic) atom – solutions of the Schrodinger equation, spectrum of the hydrogen atom
- application of quantum mechanics to multielectron atoms
- application of quantum mechanics to molecular structure
- electronic structure calculations – Hartree-Fock, post-HF methods, semi-empirical calculations, and density functional theory

CH432: BIOPHYSICAL CHEMISTRY (SEMESTER II)

Staff: Dr. David Cheung (coordinator), Dr. Mihai Lomora

1. Molecular Driving Forces
2. Analysis of Biomaterials

1. Molecular Driving Forces (12 hours, DC)

This block of lectures will explore how the behaviour of chemical and biological systems can be understood from simple physical principles. It will cover the following topics:

- Entropy and free energy
- Interfaces, wetting, and capillarity
- Phase transitions and phase separation
- Co-operativity
- Adsorption, binding, and catalysis

2. Analysis of Biomaterials (12 hours, ML)

The course outline and learning outcomes that will be assessed from this topic are as follows:

- General overview of biomaterials: types, properties, biocompatibility
- Physical, chemical, mechanical analysis (bulk and surface)
- In vitro / in vivo evaluation of biological properties
- Safety and biocompatibility assessment (standards and methods)

CH438: BIOORGANIC CHEMISTRY (SEMESTER II)

Tutors: Prof. Peter Crowley (coordinator) and Dr. Stanislas von Euw.

Sections:

1. Supramolecular Protein Chemistry – Prof. Crowley
2. TBC – Dr von Euw

1. Supramolecular Protein Chemistry (12 h)

Learning outcomes:

- Protein interactions and molecular recognition
- Macrocycles, calixarenes, cucurbiturils, cyclodextrins
- Supramolecular ligands for protein recognition and assembly
- The chemistry of the cationic residues Arg and Lys
- Methods to study protein interactions (*e.g.* X-ray, NMR, ITC)

2. TBC

Learning outcomes: TBC

CH445: ADVANCED INORGANIC CHEMISTRY (SEMESTER II)

Staff: Dr. Pau Farras (coordinator), Dr. Constantina Papatriantafyllopoulou

1. Energy and respiration in biological systems (Dr. Pau Farras)
2. Molecular Magnetism (Dr. Constantina Papatriantafyllopoulou)
3. Porous Materials (Dr. Constantina Papatriantafyllopoulou)

This module will look over contemporary chemistry, with examples of inorganic chemistry which aim to solve some of the current societal challenges. The content of this module has direct relationship with the Sustainable Development Goals (SDG):

- SDG2: No Hunger
- SDG6: Clean Water and Sanitation
- SDG7: Affordable and Clean energy
- SDG11: Sustainable Cities and Communities
- SDG13: Climate Action

1. Energy and respiration in biological systems (11 lectures + 2 tutorials, PF)

The students will be introduced to the synergy between natural and artificial systems for the design of novel metal-based devices to tackle the issues related to renewable energies.

The learning outcomes that will be assessed will include:

- Correlation between basic electron transfer theories with real biological systems such as proteins.
- Photosynthesis and mechanisms of energy transfer.
- Oxygen metabolism and fuel cells.
- Nitrogen fixation and the future of fertilisers.

2. Molecular Magnetism (6 lectures + 1 tutorial, CP)

The learning outcomes that will be assessed are:

- The student being able to understand basic concepts and definitions in molecular magnetism (magnetization, magnetic susceptibility, spin), and recognize the different types of magnetic behaviour.
- The student being able to predict all the possible spin states for a metal compound.
- The student being able to describe and understand the mechanisms of magnetic interactions.
- The student being able to understand the single molecule magnetism behaviour and its potential use in technological applications (information storage devices, quantum computing).

3. Porous Materials (6 lectures + 1 tutorial, CP)

This lecture series will deal with the synthesis, properties and applications of porous materials. Specifically, the following topics will be covered:

- classification of porous materials;
- general features of main categories of porous materials, including zeolites, activated carbon, carbon nanotubes, mesoporous silica, mesoporous alumina, etc;
- metal-organic frameworks: synthesis, properties and applications (drug delivery, gas storage/separation, catalysis, sensing, etc)

Continuous assessment in module CH445

The continuous assessment will be in the form of in-class tests during the teaching semester that will be graded. There will be tests in the week of February 6th and in the week of March 13th. The continuous assessment will contribute 20 % of the overall grade for the module.
In addition, for part 1 Energy and Respiration, group presentations will be done on the week of March 6th and will account for 5% of the overall grade for the module.

CH446: BIOINORGANIC AND INORGANIC MEDICINAL CHEMISTRY (SEMESTER II)

Staff: Dr Andrea Erxleben (coordinator), Dr Stanislas Von Euw

Topics

1. Metals in Medicine (Dr Andrea Erxleben)
2. Metalloproteins (Dr Andrea Erxleben)
3. Biomineralisation (Dr Stanislas Von Euw)

1. Metals in Medicine [12 lectures + 2 tutorials]

The learning outcomes that will be assessed will include:

- The student being able to describe the relevance of various metals in medicine. Metals covered will include: Pt, Ru, Ga, Au, Gd and various radioactive metals (e.g. Tc).
- The student being able to describe and understand the chemistry of antitumour active platinum compounds with regard to the synthesis of cis- and transplatin, coordination chemistry of Pt, trans-effect, mechanism and kinetics of ligand substitution, solution behaviour of cisplatin, reaction of cisplatin with DNA, nucleobases and amino acids, structure-activity relationships for Pt drugs, Pt NMR.
- The student being able to understand and explain aspects of the coordination chemistry of Ru, Ga, and Au relevant to the biological behaviour of these metals
- The student being able to understand and explain the function of photosensitizers in photodynamic tumour therapy.
- The student being able to understand and explain the study of covalent and non-covalent interactions between metal complexes and DNA.
- The student being able to understand and describe the generation and selection criteria of therapeutic and diagnostic radionuclides, the synthesis of radiopharmaceuticals and the function of radiosensitizers.
- The student being able to understand and explain the choice of metals and ligands suitable for MRI contrast agents.

2. Metalloproteins [6 lectures + 1 tutorial]

The student will be introduced to the role of metal ions in biological systems. Particular emphasis will be given to zince proteins and zinc enzymes and to metal complexes as their structural and functional models.

The learning outcomes that will be assessed will include:

- The student being able to present and analyse evidence that supports mechanisms of action of zinc enzymes including support for proposed intermediates
- The student being able to relate the properties of zinc to its roles in biological systems
- The student being able to represent the mode of action of metalloenzymes using catalytic cycles
- The student being able to apply the Michaelis-Menten equation to analyse kinetic data
- The student being able to describe and explain the different type of zinc sensors
- The student being able to solve unseen problems in bioinorganic chemistry

3. Biomineralisation [6 lectures + 1 tutorial]

The students will be introduced to the mechanisms of biomineralization. A particular emphasis will be given to calcified tissues (bone, mollusc shells) since their hierarchically-organized structures provide design principles for the fabrication of advanced materials.

The learning outcomes that will be assessed will include:

- The student being familiar with the concepts of biomineralization.
- The student being familiar with a number of materials characterization techniques used to investigate the growth of inorganic crystals in synthetic and biological systems.
- The student being able to describe and identify the different pathways to crystallization associated with non-classical crystal growth.
- The student being able to explain the different bio-inspired mineralization processes.

CH4113: ORGANIC CHEMISTRY (SEMESTER II)

Staff: Dr Eddie Myers (coordinator), Prof. Paul Murphy

1. Pericyclic and Radical Reactions (12 h)
2. Selectivity in Organic Synthesis (12 h)

1. Pericyclic and Radical Reactions (12 h)

Students will be assessed on the following learning outcomes:

- The ability to classify a pericyclic reaction as either a cycloaddition, an electrocyclic reaction, a sigmatropic rearrangement or a group-transfer reaction.
- The ability to predict the sense of a pericyclic reaction (suprafacial/antarafacial and disrotatory/conrotatory) under a certain set of reaction conditions (thermal/photochemical) based on the Woodward–Hoffman Rules.
- The ability to draw a set of π-based molecular orbitals for any conjugated molecule, to assign electrons to these orbitals, to identify the HOMO and LUMO orbitals and to use the resulting information to predict the sense of a pericyclic reaction under thermal or photochemical conditions.
- To understand the concept of stereospecificity pertaining to pericyclic reactions and to be able to predict the diastereoselectivity of a pericyclic reaction.
- The ability to use structural features to predict the relative rate and regioselectivity of pericyclic reactions.
- The ability to draw radical reaction mechanisms by using single-headed (fishhook) arrows.
- To understand and distinguish radical stability and reactivity.
- To understand the major types of reactions and processes involving radicals, such as fragmentation of weak bonds to form radicals, atom abstraction reactions, the addition of radicals to alkenes, and radical-radical combination and disproportionation.
- To understand radical chain processes and their use in the formation of rings and polymers
- To understand electron paramagnetic resonance as an analytical method for the study of radicals
- To have an appreciation for the role of radical reactions in biology and chemical biology.

2. Selectivity in Organic Chemistry (12 h)

The learning outcomes that will be assessed will include evaluation of student's knowledge and understanding of important reactions in organic synthesis and factors which influence those such as for those mentioned below:

- Chemoselective reactions of carbonyl compounds with various reducing reagents.
- Chemoselective reactions of alcohols and alkenes with oxidising agents
- Stereoselective olefination (alkene forming reactions)
- Enantioselective oxidation and reduction
- Stereoselective substitution reactions (basis in SN1, SN2 reactions)
- Regioselective reactions with carbohydrates/cyclic epoxides
- Bioorthogonal reactions

CH4101: RESEARCH INVESTIGATION

All students will undertake a research investigation. Information on the research project topics are given in this booklet. Students will submit their preferences by 12 noon on Friday 15th July 2022 and assignments will then be based on 3rd year Chemistry grades.

Learning outcomes from this module are provided below:

Students will manage their own learning.
Students will apply the basic knowledge gained earlier in the programme in order to consolidate and extend their knowledge and understanding of chemistry.
Students will become integrated into a scientific research team and develop teamwork skills.
Students will also develop skills such as finding data or information from the literature, to organise and summarise this and to present the outcomes of their investigations, placing it in context.

More specifically students will:

1. Establish or become aware of the state of the art in assigned topics
2. Critically analyse data or facts obtained from library and/or laboratory work
3. Use the facts or data obtained by this independent investigation to challenge current teaching and/or myths/hyperbole and/or to provide new insights and/or advance a topic in Chemistry
4. Demonstrate a greater understanding and knowledge within Chemistry as a result of their independent investigation
5. Demonstrate competence in recording, reporting & presenting the outcomes of their independent investigative work
6. Participate in the research team activities
7. Be able to carry out and report their research in an ethical manner

SCHEDULE FOR RESEARCH INVESTIGATION MODULE

- See timetable for workshops in health & safety and literature & database searching. The instructors will inform you of the deadlines for submission of assignments related to these aspects. *Marks will be deducted for any late submissions*

- The laboratories will be open for the research from **Monday 5th September 2022** until **Friday 18th November 2022**

  For health and safety reasons, undergraduates are restricted in the laboratory between 9am-6pm on Monday-Friday and should never work alone.

  Chemistry students are expected to work ~25h per week generating data on their project in this period.

- Students will keep a lab notebook to document their experiments, observations, and provide a preliminary interpretation of the results, as well as include information about the experiments risk assessment. *An electronic copy of the lab notebook will be submitted to your supervisor no later than* ***Thursday 8th December 2022 by 15.00*****.**

- Students are strongly encouraged to keep a research journal. This will be beneficial for research planning and goals achievement. It will provide evidence about the project/student's progress in a timely manner and can act as a self-assessment tool. An electronic copy of the research journal template can be downloaded from blackboard. Copies of the research journal will be submitted to supervisor *no later than* ***Thursday 8th December 2022 by 15.00*****.**

- Students are assigned a second reader of their project reports. Students should meet their second reader twice during the project to discuss their progress. Meetings will be held on ***5th October*** and ***16th November 2022***. Students will confirm the time and venue of the meeting with their second reader. PowerPoint slides will be submitted to the second reader at least 3 days in advance of each meeting.
  Meeting 1 agenda: a brief literature review, project aim and preliminary results.
  Meeting 2 agenda: research update and dissertation outline.

- Students are assigned a third reader of their project reports. The role of the third reader will be to assess the quality of the report according to the marking scheme on page 26.

- Upload electronic copy of the project thesis is required no later than **Thursday 8th December 2022 by 15.00**– *Marks will be deducted for late submission.*

- Oral and poster presentations on projects will take place in the week of **12th December 2022**. The oral presentations will be assessed by the academic staff attending. The poster presentations will not be graded. Students will have the opportunity to share their efforts and results with their fellow students and academic staff. It will be a part of a celebratory research day marking the completion of the research projects.

- Students can revise the project report taking on board the comments raised by the 1st and 2nd reader and the academic staff attending the project presentation. An electronic copy of the revised report is required to be uploaded no later than one week after the date of presentation.

FEEDBACK ON REPORTS

Students should arrange an appointment with their supervisors to obtain feedback on a draft of the write-up of the research report. Please provide a timely draft to your supervisor in advance of this meeting (at least one week in advance) and please confirm the time and date of this meeting with your project supervisor in advance.

RESEARCH JOURNAL TEMPLATE

WEEK 1 (5/9/2022)	
Goal(s)/associated tasks:	
Completed tasks:	
Reflective entry:	

An electronic copy of the template can be downloaded from blackboard

GUIDELINES FOR STUDENTS IN WRITING A SYNTHESIS PROJECT REPORT

1. Title of Project

2. Summary or Abstract
A concise summary (up to 350 words) of what has been achieved. This should be explicit and reference should be made to work/experiments carried out and the results. Highlights from the research should specifically be included. A graphic is recommended to support this abstract.

3. Introduction
Approximately 4-8 pages (A4, typed, one and a half or double line spacing, margins approx 1", font such as Times and font size 12). Structure diagrams or schemes can be drawn with ChemDraw available for all students. The introduction should include background to the project, explaining the reasons for undertaking the work and include a project plan. In the case of synthetic projects for example, this could show a scheme. References must be included and usually are numbered in sequence as they are found in text with a superscript and the full reference listed at the end of the report.[1-3] Compounds should be numbered (**in bold**) as they appear in schemes. The final section of the introduction should outline the aims of the project. The final sentence or paragraph should summarise what has been achieved.

4. Results and Discussion

Students are advised to give a concise presentation of results presented first followed by a discussion of their significance (novelty of method?, novel mechanism?). Please also provide any relevant figures or schemes or tables that are needed to efficiently and clearly present your results.

In synthetic projects, there is no need to provide mechanisms for all reactions (although you will be expected to be able to discuss these during the oral assessment). Please only discuss a mechanism if an unexpected product is obtained or if this is central to the project objective.

When relevant there can be a description of the key characterisation data that supports a structural assignment, a brief description of how the reactions were carried out and yields can be given etc.

Example from a synthesis report: "The bromide derivative (**10**) was obtained (65%) after treatment of penta-O-acetyl-α-D-glucopyranose with hydrogen bromide in acetic acid. The ^{1}H-NMR spectrum of **10** had signals at δ 6.30 (1H, d, *J* 4.0 Hz, H-1), 4.80-3.50 (6H, ms, H-2–6) and 2.00-2.10 (12H, 4 x s, CH_3C=O), which were in excellent agreement with literature data.[4]" Tables can be used and diagrams/reaction schemes should be included and numbered etc. (Scheme 1, Fig. 1, Table 1).

Compounds should be numbered in order of appearance in schemes etc. If NMR is not relevant, then give X-ray or other spectroscopic data or analytical data to support your assignments.

5. Conclusions
Please include a conclusions section, summarizing briefly the main findings of the project.

6. Experimental
Description of experiments should be given in detail sufficient to enable experimental workers to repeat them.

For synthesis projects include full characterisation, yields, m.pt., R_f, NMR data, IR data, $[\alpha]_D$, microanalysis (for new compound), mass data and their assignments should be included). If a compound is not new, please include a citation to where it has been characterized previously and include some characterization data (e.g. ^{1}H-NMR, IR, LRMS and alpha-D) and state that the data is in good agreement with that described previously. You may include a general experimental section if this is relevant.

Typical experimental procedure (for a synthesis project) for a new compound and assignment of analytical data:

***N*-(2,3,4,6-Tetra-*O*-acetyl-(β-*D*-glucopyranosyl)-5-ethylthiophene-2-carboxamide 9** The reaction of 5-ethylthiophene-2-carboxylic acid (0.23 g, 1.44 mmol) as described for 3-bromothiophene-2-carboxylic acid gave a mixture of anomers (0.64 g, 91 % yield, α:β, 1:16). The residue was recrystallised from EtOAc and cyclohexane to afford β-anomer **9** as a colourless crystalline solid (0.42 g, 51%) and as an adduct with EtOAc (1:1); mp 64-66 °C; $[\alpha]_D$ +12 (*c* 8.0, $CDCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 (1H, d, *J* 3.9 Hz, aromatic H),

6.84 (1H, d, $J_{NH,H1}$ 9.3 Hz, NH), 6.77 (1H, dd, *J* 3.9 Hz, *J* 0.9 Hz, aromatic H), 5.37 (2H, 2 x overlapping t, *J* 9.3 Hz, H-1,3), 5.10 (1H, t, *J* 9.3, H-4), 5.03 (1H, t, *J* 9.3 Hz, H-2), 4.34 (1H, dd, $J_{6a,6b}$ -12.5 Hz, $J_{6a,5}$ 4.2 Hz, H-6a), 4.09 (1H, dd, $J_{6b,6a}$ -12.5 Hz, $J_{6b,5}$ 2.1 Hz, H-6b), 3.88 (1H, ddd, $J_{5,4}$ 9.9 Hz, $J_{5,6a}$ 4.2 Hz, $J_{5,6b}$ 2.1 Hz, H-5), 2.86 (2H, q, *J* 7.5 Hz, CH_2CH_3), 2.08, 2.04 (2s), 2.03 (each 3H, each s, each CH_3), 1.32 (3H, t, *J* 7.5 Hz, CH_2CH_3); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.5, 170.7, 169.9, 169.6 (each ester C=O), 161.8 (amide C=O), 154.9, 134.3 (each aromatic C), 129.5, 124.6 (each aromatic CH), 78.9, 73.6, 72.6, 70.7, 68.3 (each CH), 61.7, 23.8 (each CH_2), 20.6, 20.7, 15.7 (each CH_3); ESI-LRMS *m/z* 486 $[M+H]^+$, 324, 271, 169; ESI-HRMS (*m/z*) calcd for $C_{21}H_{28}NO_{10}S$ 486.1434, found *m/z* 486.1448 $[M+H]^+$. Anal Calcd for $C_{25}H_{35}NO_{12}S$ (EtOAc adduct): C, 52.35; H, 6.15; N, 2.44; S, 5.59. Found: C, 52.22; H, 6.09; N, 2.49; S, 5.92.

Include the name of the compound, if possible. Many compounds can be named by checking for related compounds in SciFinder and using names provided in SciFinder abstracts as guidelines. Chemdraw can also be helpful in naming. Please consult your supervisor for advice on preparation of the experimental section. This can vary significantly between research areas.

Note: You can use Reaxys (www.reaxys.com) or SciFinder to search for compounds to determine whether they are new or known. If a compound is known then a citation should be provide. If analytical data is in agreement with data reported previously then this should be stated. Do include melting points and alpha D data if relevant and do state the literature data for these, if relevant.

7. References (Please use a standard style such as the one (RSC) outlined below).

1. I. Fleming, *Frontier Orbitals and Organic Chemical Reactions,* Wiley, Chichester, 1976, p. 55.
2. A. J. L. Beckwith and K. U. Ungold, in *Rearrangements in Ground and Excited States,* ed. P. de Mayo, Academic Press, New York, 1980, vol. 1, p. 161.
3. P. D. Cunningham, N. W. A. Geraghty, P. J. McArdle, P. V. Murphy and T. J. O' Sullivan, *J. Chem. Soc., Perkin Trans. 1*, 1997, 1.
4. H. Kessler and M. Hoffmann, *J. Am. Chem. Soc.* 1994, **118**, 10156.
5. X. Y. Smiths, *Journal of Flame,* 2000, **22**, 10157.

Reference 1 is a typical book, Reference 2 is typical for a chapter in an edited book. References 3 and 4 are typical journal references.

8. Appendix

You should include any relevant spectra, chromatograms etc. For example for projects using organic synthesis you may include ^{1}H and ^{13}C NMR spectra for any new compounds as evidence of homogeneity of purity of compounds you prepare. You may include a **compound characterization checklist** in your report. This corresponds to a table where you indicate the analysis you obtained on each compound.

9. Project risk assessment

Please include your project risk assessment as this will be evaluated as part of the project work. This should be signed by the student and supervisor and have identified major hazards assocated with project work.

10. Plagiarism. The thesis should be written in your own words and not copied from any reviews or internet. If reproducing any figures from the literature in the thesis then please obtain copyright permissions and cite the original article. Obtaining copyright permissions can usually be done online where the article is originally published. Plagiarism must be avoided. See NUI Galway guidelines on plagiarism at http://www.su.nuigalway.ie/site/view/313/. Action will be taken by the examiners when plagiarism is found to occur.

Grading of project and the write-up will be based on strict adherence to guidelines provided herein.

The number of total pages does not normally need to exceed 35 pages. The student is recommended to focus on the quality of their report.

GUIDELINES FOR THE PROJECT REPORT (Measurement or Modelling Projects)

1. Title of Project: (Name, supervisor etc.)

2. Summary or Abstract

A concise summary (up to 350 words) of what has been achieved. This should be explicit and reference should be made to work/experiments carried out, results obtained, and the significance of these results. Highlights from the research should be specifically included. Inclusion of a graphic is recommended.

3. Introduction

Approximately 4-8 pages (A4, typed, one and a half line spacing, margins approx 2.5 cm, font such as Times and font size 12). Structure diagrams or schemes can be drawn with ChemDraw available for all students. The introduction should include background to the project, explaining the reasons for undertaking the work and include a project plan. References must be included and usually are numbered in sequence as they are found in text with a superscript and the full reference listed at the end of the report.[1-3] The final section of the introduction should outline the aims of the project. The final sentence or paragraph should summarise what has been achieved. The introduction should be written in your own words and not copied from any reviews or internet. If reproducing any figures from the literature in the thesis then please obtain copyright permissions and cite the original article. This can usually be done online where the article. Plagiarism must be avoided. See NUI Galway guidelines on plagiarism at http://www.su.nuigalway.ie/site/view/313/

4. Experimental

Description of experiments should be given in detail sufficient to enable experimental workers to repeat them. Include full details of the samples you studies, where they were obtained, how stored and handled. Include full details of the instrumentation and software used. Explain clearly how you collected you data and what instrumental parameters were used.

All the experimental data and procedures should reference the appropriate pages in your laboratory notebook which should be submitted to the supervisor with the final draft for cross referencing purposes.

Typical experimental procedure (for an analytical project):

Instrumentation and data collection: Raman measurements were performed in triplicate at room temperature using an Avalon Instruments Raman spectrometer with 785 nm excitation. A laser power of ~70 mW at the sample was used and spectra were collected with a resolution of 8 cm^{-1} and a typical exposure time of 10 s. For solution samples, stainless steel 96-well plates were used and multiple spectra were collected from a 3 × 3 grid (0.5 mm spot spacing) from which a single averaged spectrum was generated for data analysis. Fluorescence measurements were made at 25°C with a Cary Eclipse (Varian) fluorimeter using procedures previously described. Yeastolate samples were randomly removed from storage, defrosted at room temperature and allowed to reach room temperature, and handled using aseptic techniques. For each solution, 1 ml was pipetted into a cuvette and sealed before allowing to thermally equilibrate for several minutes prior to measurement. Spectral SERS data was pre-processed to reduce the influence of baseline drift, scatter effects, and uncontrolled fluctuations. Spectra containing cosmic interference were discarded prior to averaging of the spectra. The average spectrum was then treated with a multiplicative scatter correction, then an asymmetric weighted least squares algorithm to remove baseline offsets before finally applying a background correction using an orthogonal projection procedure. For SERS-ROBPCA analysis, the first derivative (SavGol) method was then implemented to further reduce measurement/instrumental effects and accentuate analyte signals. For EEM-MROBPCA analysis, Rayleigh and Raman scatter were removed from EEM data by replacing with a curve fit, connecting points either side of the bands using imputation. All calculations were performed using MATLAB ver. 7.4, PLS_Toolbox 4.0, and in-house-written toolboxes.

Please consult with your supervisor for advice on preparation of the experimental section. This can vary significantly between research areas. It is good practice to look at the style and content of peer-reviewed journals to assist in preparing your project.

5. Results and Discussion
Students are advised to give a concise presentation of results presented first followed by a discussion of their significance (novelty of method?, novel data?). In modelling projects, there is no need to provide detail of any code used (this can be included in an appendix).
In analytical type projects there is no need to include every spectrum etc., show an indicative or important example then summarise the important results in overlay plots or tables. If you have a lot of important data place it in an appendix with a brief description of the data. You can then refer to this appendix in your text. When relevant there should be a comparison between your data/results and relevant examples from the literature, *e.g.* are your spectra the first to show a new species? Is your data better quality than what's been published? If so, how so? Look at peer-reviewed papers for examples of how this is done professionally.

6. Conclusions
Please include a conclusions section (1-2 pages), summarizing your main achievements.

7. References (Please use a standard style such as the one outlined below).
[1] J. R. Lakowicz, Principles of Fluorescence Spectroscopy, 3rd Edition ed., Springer, New York, 2006.
[2] T. Cartwright, G. Shah, Culture media, in: J.M. Davis (Ed.) Basic Cell Culture, Oxford University Press Inc., New York 2002, pp. 69-106.
[3] P. W. Ryan, B. Li, M. Shanahan, K. J. Leister, A. G. Ryder, Prediction of Cell Culture Media Performance Using Fluorescence Spectroscopy, *Anal. Chem*., 82 (2010) 1311-1317.
[4] PLS_Toolbox, ver. 2.0, Eigenvector Research Inc., 3905West Eaglerock Drive,Wenatchee,WA.

Reference 1 is a typical book, Reference 2 is typical for a chapter in an edited book. Reference 3 is a typical journal reference, and 4 is for referencing software.

8. Appendix
In addition to the above you will need to include your project research assessment. You should include any relevant collections of spectra, modelling code, repeat experiments etc. here.

9. Project risk assessment
A risk assessment has to be carried out for all projects, including theoretical or computer-based projects. In certain cases, no risks may be identified (e.g. computational projects) and this can be stated on the risk assessment form.

10. Plagiarism. The thesis should be written in your own words and not copied from any reviews or internet. If reproducing any figures from the literature in the thesis then please obtain copyright permissions and cite the original article. Obtaining copyright permissions can usually be done online where the article is originally published. Plagiarism must be avoided. See NUI Galway guidelines on plagiarism at http://www.su.nuigalway.ie/site/view/313/. Action will be taken by the examiners when plagiarism is found to occur.

Grading of project and the write-up will be based on strict adherence to guidelines provided herein.

The number of total pages does not normally need to exceed 35 pages. The student is recommended to focus on the quality of their work and report.

GUIDELINES FOR STUDENTS IN WRITING A NON-LABORATORY BASED REPORT

In the event that a student is assigned to a research investigation where much of the work and obtaining data or facts is carried out in the library and/or by working with data available to the supervisor then there is scope to modify the structure of the report. It is advisable that the student discuss the structure of the write up with the supervisor. The following sections must still be included in the report.

1. Title of Project: (see below for format which should be used)

2. Summary or Abstract
A concise summary (up to 350 words) of the objectives, findings and conclusions. Please include any particular highlights which emerged from the investigative work.

3. Introduction
This should be typed, one and a half or double line spacing, margins approx 1", font such as Times and font size 12). Structure diagrams or schemes can be drawn with ChemDraw available for all students. The introduction should include background to the investigation, explaining the reasons for undertaking the work and include objectives. References must be included and usually are numbered in sequence as they are found in text with a superscript and the full reference listed at the end of the report.[1-3] Compounds should be numbered (**in bold**) as they appear in schemes. The final section of the introduction should outline the aims of the investigation. The introduction should be written in your own words and not copied from any reviews or the internet. Plagiarism must be avoided. See NUI Galway guidelines on plagiarism at http://www.su.nuigalway.ie/site/view/313/ and the appropriate section in this booklet.

4. Presentation and Discussion of findings

Students are advised to detail their findings of their investigative work which is based on data available to the host supervisor and as a result of library and literature investigations. This should be followed by a discussion of their significance (novelty of method?, novel mechanism?). Please also provide any relevant figures or schemes or tables that are needed to efficiently and clearly present your results. Compounds should be numbered in order of appearance in schemes etc.

5. Conclusions
Please include a detailed conclusions section.

6. References (Please use a standard style such as the one (RSC) outlined below).
1. I. Fleming, *Frontier Orbitals and Organic Chemical Reactions,* Wiley, Chichester, 1976, p. 55.
2. A. J. L. Beckwith and K. U. Ungold, in *Rearrangements in Ground and Excited States,* ed. P. de Mayo, Academic Press, New York, 1980, vol. 1, p. 161.
3. P. D. Cunningham, N. W. A. Geraghty, P. J. McArdle, P. V. Murphy and T. J. O' Sullivan, *J. Chem. Soc., Perkin Trans. 1*, 1997, 1.
4. H. Kessler and M. Hoffmann, *J. Am. Chem. Soc.* 1994, **118**, 10156.
5. X. Y. Smiths, *Journal of Flame,* 2000, **22**, 10157.

Reference 1 is a typical book, Reference 2 is typical for a chapter in an edited book. References 3 and 4 are typical journal references.

Grading of project and the write-up will be based on strict adherence to guidelines provided herein.

ASSESSMENT OF THE RESEARCH INVESTIGATION

	Areas where the project is assessed	Mark (out of 100)	Weight	Grades awarded must be justified below
Completed by 3rd Reader	Style, appearance, organisation and English usage. Organisation of data/results	0	5.0%	
Completed by 3rd Reader	Clarity of introduction - appropriateness of references - setting the project in context	0	10.0%	
Completed by 3rd Reader	Results, discussion and experimental	0	20.0%	
Completed by 3rd Reader	Conclusions, suggestions for future work	0	5%	
	Computed grade for the report by the 3rd Reader	0	out of 40	
	Computed grade for the report by the 2nd Reader (see marks on right)	0	out of 40	
	Average grade/35 for the report based on 1st and 2nd Reader	0	out of 40	
Completed by 2nd Reader	**2nd Reader assessment after two meetings with the student.** How well prepared was the student for the meetings? How competent were they in discussing their project and in their ability to answer questions raised by the second reader?	0	5%	
Completed by Supervisor	**Supervisor's evaluation of standard of research work and student's productivity:** Was the recording of data, spectra, laboratory book etc. to a high standard? Consider the standard of the experiments carried out during the course of the work. Quality and quantity of results/data/outputs generated in the time available. Consider the development of team work skills and the level of difficulty of the project in terms of generating results.	0	25.0%	
Completed by Supervisor	**Supervisor's assessment of intellectual contribution to the project:** for example, assess the student's independence and ability to address problems or challenges that arose during the project work, or to learn from their mistakes or from experiments they carried out that were not very successful.	0	10.0%	
	Computed Grade for project performance	0	out of 35	
agreed mark from those present at the presentation	**Oral Presentation:** Organisation & delivery, slide quality, & answering of questions weighted equally	0	20.0%	
	Originality/Plagiarism. Any concerns?		y/n	
	Research journal		y/n	
	Submission of revised report		y/n	
	Poster presentation		y/n	
	Final Grade	0		

2nd Reader

	Areas where the project is assessed	Mark	Weight	Grades awarded must be justified below
Completed by 2nd Reader	Style, appearance, organisation and English usage. Organisation of data/results	0	5.0%	
Completed by 2nd Reader	Clarity of introduction - appropriateness of references - setting the project in contex	0	10.0%	
Completed by 2nd Reader	Results, discussion and experimental	0	20.0%	
Completed by 2nd Reader	Conclusions, suggestions for future work	0	5%	
	Computed grade for the report by the 2nd Reader	0	out of 40	

PLAGIARISM

Plagiarism is the act of copying, including, or, directly quoting from the work of another, without adequate acknowledgement, in order to obtain benefit, credit or gain. Plagiarism can apply to many materials, such as words, ideas, images, information, data, approaches or methods. Sources of plagiarism can include books, journals, reports, websites, essay mills, another student, or another person.

Self-plagiarism, or auto-plagiarism, is where a person re-uses work previously submitted to another course within the University or in another Institution or even a journal. Plagiarism can also involve overly relying on a source – even if it is referenced correctly.

All work submitted by students is accepted on the understanding that it is their own work and contains their own original contribution, except where explicitly referenced using the accepted norms and formats of the appropriate academic discipline. Students are required to sign an affidavit to confirm the above for all submissions in fourth year chemistry.

NUI Galway applies a penalty grid to plagiarised submissions. All relevant information can be found at: www.nuigalway.ie/plagiarism. This penalty grid is University policy and no exceptions will be made.

Supervisor responsibilities

Supervisors will encourage students to avoid plagiarism during all meetings where preparation of project reports etc. are being discussed.

Plagiarism advisor responsibilities

The plagiarism advisor will check all submissions using Turnitin. In cases of plagiarised work, the plagiarism advisor will determine if there is a case to be made. If the decision is positive, the fourth year examiners including the supervisor and second reader will be contacted and appropriate action taken. The plagiarism advisor will write a confidential report, recording the decision and any penalty.

Student responsibilities

All students will be given access to their own Turnitin report. In cases of plagiarised submission, students will be obliged to formally meet with their project supervisor to discuss the plagiarised submission. The *final project report* will be submitted electronically through Blackboard and Turnitin. In cases of plagiarised submissions the plagiarism advisor and the 4th year committee will be contacted and they will decide if appropriate action will be necessary according to University policy (www.nuigalway.ie/plagiarism).

Plagiarism adviser

Plagiarism adviser is Dr. Pau Farras.

AFFIDAVIT

Student Declaration on Plagiarism, Collusion or Copying

This declaration is to be completed and signed by the **student**. It must be included in the essay, first and final draft of the project reports.

I declare that this material, which I now submit for assessment, is my own work and that any assistance I received in its preparation is fully acknowledged and disclosed in the document. To the best of my knowledge and belief, all sources have been properly acknowledged, and the assessment task contains no plagiarism.
I understand that plagiarism, collusion, and/or copying are grave and serious offences and am aware that penalties could include a zero mark for this assessment, suspension or expulsion from NUI Galway. I have read the NUI Galway code of practice regarding plagiarism at www.nuigalway.ie/plagiarism.
I acknowledge that this assessment submission may be transferred and stored in a database for the purposes of data-matching to help detect plagiarism. I declare that this document was prepared by me for the purpose of partial fulfilment of requirements for the programme for which I am registered with the AUA. I also declare that this assignment, or any part of it, has not been previously submitted by me or any other person for assessment on this or any other course of study or another college.

_____

Student Name

_____ _____

Student Signature Date

IMPORTANT:

Please sign and return to School Office (Karen.kelly@nuigalway.ie) by Wednesday 7th September 2022

Treatment of Personal Data*

I am aware that if I submit a medical certificate/letter regarding absences and/or any other personal information, this information may be shared with staff of the University and examiners for purposes related to assessing and maximizing my academic performance.

Signature _____

* *If you have issues which you would prefer to remain confidential to the recipient it must be clearly stated. Be aware this will limit the School's ability to react to or consider such information when assessing performance.*