School of Physical and Chemical Sciences

UNIVERSITY OF CANTERBURY
Te Whare Wānanga o Waitaha
CHRISTCHURCH NEW ZEALAND

General Course Information

PROD 235
Formulation Chemistry

0.1250 EFTS 15 Points
First Semester 2022

Prescription
Chemistry related to product formulation, including common organic chemical structures and reactivity; separation, purification and characterisation of chemical compounds; the function and structure of surfactants and micelles; the chemical basis of dyes, colourants and fragrances; and an introduction to intellectual property considerations for new chemical compounds and formulations.

Description
This course is required for Bachelor of Product Design students majoring in Chemical Formulation Design.

The topics covered by this course are:

- Organic Chemistry
- Separation, Purification and Characterisation methods
- Detergents, Surfactants and Micelles
- Dyes and Colouring
- Fragrance Chemistry and the Sense of Smell
- Trade Secrets, Patents and Intellectual Property

Timetable
Lectures: Three hours of lectures per week. Details to be confirmed on 'My Timetable' and the web.
Tutorials: Tutorials will be scheduled as required and arranged by the Lecturer of each course block.

Students should note that in the Science Faculty the average student is responsible for approximately 3.2 hours of additional study for each hour of lecture at the 200-level.

Course Co-ordinator
Dr Tim Allison, School of Physical and Chemical Sciences
Beatrice Tinsley 328, Email: timothy.allison@canterbury.ac.nz
Email me if you have any queries about the course.

Assessment

BestChoice:	5%
Test 1:	22.5%
Test 2:	22.5%
Final examination:	50%

Examination and Formal Tests
Tests: 1.5 hours, details to be advised
Exam: 2.5 hours, details to be advised

Prerequisites
CHEM 111. In addition, CHEM 112 is a *strongly recommended* background course. RP: BIOL 111 or PROD 131.

Web-based resources
Various learning resources for this course are available via the University of Canterbury's *Learn* web site -- http://learn.canterbury.ac.nz/. This site will also be used regularly as a means of communication and information distribution for all of your Canterbury courses. You should familiarise yourself with *Learn* as soon as possible.

Goal of the Course

- This course will introduce BProdDesign students to several aspects of Chemistry relevant to formulated products. These will include basic Organic, Surfactant and Micelle Processes, Fragrance Chemistry, Separation and Characterisation Methods, and relevant Intellectual Property topics.

Learning Outcomes (see also detailed Learning Objectives after Course Content, below)

- Have a working understanding of the fundamental organic chemistry including the three dimensional structure of molecules and general reactions of various functional groups.
- Understand what colloids, surfactants and micelles are, and how surfactants are important in commercial polymerization processes.
- Develop understanding of the theory and basic application aspects of a variety of characterisation methods (chromatography, mass spectrometry, nuclear magnetic resonance and other selected spectroscopic techniques).
- Understand how chemical compounds can be separated and purified through common methods such as extraction, distillation, crystallisation, etc.
- Be able to describe the origin of colour in molecules, how products are colourised and how colours are made fast, including traditional products from Māori and Pasifika
- Understand the physiological basis of smell, the chemical basis of odour and how chemical compounds can be blended to create fragrances
- Be conversant with issues related to patenting and intellectual property for new chemical compounds and formulations, including those based upon traditional compounds

Summary of the Course Content

BLOCK 1: (12 lectures/tutorials)

Essentials of Organic Chemistry for Formulation Chemistry
This part of the course will introduce you to the important fundamentals of organic chemistry. You will learn how to represent the structures of organic compounds in three dimensions, how molecules can exist in different conformations and as different stereoisomers. The common functional groups found in organic chemistry will be discussed along with the general types of reactions that they undergo. A basic introduction to the way we represent reaction mechanisms will also be covered.
Lecturer: **Zach Stueven, zachariah.stueven@pg.canterbury.ac.nz**

BLOCK 2: (12 lectures/tutorials)

Separation, Purification and Characterisation Methods for R&D and QA
The separation, purification and characterisation of compounds and mixtures, on both large scales and small, are critical steps in industrial research and development and in quality assurance processes.
The following laboratory and instrumental techniques will be covered:

- Extraction, Distillation, Crystallisation, Chromatography (TLC, column, GC, HPLC), Nuclear Magnetic Resonance, Mass Spectrometry

These lectures will introduce the principles of these characterisation methods, relevant instrumentation and outline selected applications. These methods are commonly used in many industrial, environmental and forensic laboratories. Basic understanding of the fundamentals behind such methods, and simple practical aspects of their application to solving chemical problems relevant to R&D and QA is an important component of training of formulation professionals in these areas.
Lecturer: **Dr Tim Allison, Beatrice Tinsley 328, timothy.allison@canterbury.ac.nz**

BLOCK 3: (4 lectures/tutorials)

Surfactants and Polymerization
Firstly we look at colloids, surfactants and micelles – what are they, how are they similar, how are they different? Then we look at polymerization involving surfactants, viz. emulsion polymerization and suspension polymerization.
Lecturer: **A/Prof. Greg Russell, Beatrice Tinsley 322, greg.russell@canterbury.ac.nz**

BLOCK 4: (8 lectures/tutorials)

Dyes and Colouring
The importance of colour in a consumer product. An overview of the biology, chemistry and physics of the three fundamentals of colour; colour perception; illumination source (light and the electromagnetic spectrum) and the colour producing properties of object it interacts with (the origins of colour in molecules). An overview of colourant classification with examples of uses of colourants in products of different kinds (lipsticks, paints, polymers, dyes). Analysing colourants. Desirable properties of colourants including stability and consistency, detail on the reactions of dye molecules, achieving colour fastness and ways of fixing colour. Natural dyes and pigments, particularly in the context of tikanga Māori.
Lecturer: **Dr Jodie Johnston, Beatrice Tinsley 325, jodie.johnston@canterbury.ac.nz**

BLOCK 5: (8 lectures/tutorials)

The Chemical Basis of Fragrance and the Sense of Smell
The physiological mechanism of smell. Structure-odour relationships. Molecular shape and volatility and their importance in fragrance/smell. Perfume mixtures and their complexity. Design and manufacture of fragrance ingredients.
Lecturer: **Dr Jodie Johnston, Beatrice Tinsley 325, jodie.johnston@canterbury.ac.nz**

BLOCK 6: (4 lectures/tutorials)

Green Chemistry
A key issue with chemical technology is the generation of chemical waste and the utilization of hazardous substances. These challenges have led to the area of green chemistry: the design of chemical products and processes that minimize the use and generation of hazardous substances. Green chemistry seeks to reduce and prevent pollution at its source by consideration of the entire life cycle of a product, from its feedstock materials and sustainability through to waste generation and decomposition products. This course will focus on aspects relevant to formulation and product design: sustainability, health and environmental impacts.
Lecturer: **Associate Professor Owen Curnow, Beatrice Tinsley 420, owen.curnow@canterbury.ac.nz**

LEARNING OBJECTIVES

BLOCK 1:
At the end of this lecture block you should be able to:

- Draw organic molecules in three dimensions using appropriate representation.
- Describe the different types of isomerism that are possible for organic molecules.
- Explain the importance of electron delocalisation, resonance, acidity and basicity in organic molecules.
- Describe the important functional groups commonly found in organic and biological molecules.
- Classify organic reactions into specific reaction types.
- Explain the importance of various carbon compounds involved in personal care formulations.
- Understand the relevant chemical processing methods involved in formulating personal care products.

BLOCK 2:
At the end of this block, you should be able to:

- Explain the principles underlying extraction, distillation, and crystallisation
- Describe how chromatography can be used for the separation of analytes and assessment of purity
- Describe the basic principles of Mass Spectrometry
- Describe the basic principles of Nuclear Magnetic Resonance spectroscopy
- Interpret basic characterisation spectra
- Identify unknown molecular structures using complementary data provided by several characterisation methods.

BLOCK 3:
At the end of this block, you should be able to:

- Describe the molecular characteristics of surfactants
- Discuss the stability of micelles, colloids and suspensions, and how changes in conditions can affect this stability
- Outline the major features of emulsion and suspension polymerization, and in particular how surfactants play a critical role

BLOCK 4:
At the end of this block, you should be able to:

- Explain why colour is a perception and describe briefly the biology behind colour perception by the eye
- Describe the properties of light that are relevant to colour chemistry and explain how they are relevant
- Explain why objects and molecules are coloured (i.e. dispersion, diffraction, absorption, fluorescence, phosphorescence) and how that colour can be measured
- Be able to explain how colourants are classified and give examples of different colourant types and their uses in different materials
- List the desirable properties of colourants, and explain how these are assessed, why they are desirable and how they can be manipulated by certain processes (e.g. colour fastness, colour fixation)

BLOCK 5:
At the end of this block, you should be able to:

- Explain the current biological and biochemical understanding of odour perception
- Discuss the importance of stereochemistry and 3D shape for both odorants and biological macromolecules involved in the process
- Describe and give examples of chemicals that contribute to odour
- Give examples of molecules used in fragrances and perfume
- Comment on the complexity of such mixtures

BLOCK 6:
At the end of this block, you should be able to:

- Identify the grand challenges of green chemistry and consider what it will take to resolve them.
- Define “green chemistry” and place its birth and expansion in an historical context.
- Introduce the principles of green chemistry, outline examples, and establish the arguments for our need to recognize green criteria in the practice of chemistry and product design.
- Present examples of successful green technologies.
- Explain the history of certain pollutants and their impact on human health.

GENERAL INFORMATION 2022

Chemistry Department Policy on 'Dishonest Practice'
The University has strict guidelines regarding 'dishonest practice' and 'breach of instructions' in relation to the completion and submission of examinable material. In cases where dishonest practice is involved in tests or other work submitted for credit a department may choose to not mark such work ('Academic Integrity and Breach of Instruction Regulations').

The Department of Chemistry upholds this policy. It considers plagiarism, collusion, copying, and ghost writing to be unacceptable and dishonest practices:

- ***Plagiarism*** is the presentation of any material (text, data or figures, on any medium including computer files) from any other source without clear and adequate acknowledgement of the source.
- ***Collusion*** is the presentation of work performed in whole, or in part, in conjunction with another person or persons, but submitted as if it has been completed by the named author alone. This interpretation is not intended to discourage students from having discussions about how to approach an assigned task and incorporating general ideas that come from those discussions into their own individual submissions, but acknowledgement is necessary.
- ***Copying*** is the use of material (in any medium, including computer files) produced by another person or persons with or without their knowledge and approval. **This includes copying of the lab reports (raw data may be shared within the group if permitted or required by the experiment) - data analysis and interpretation of obtained results MUST be performed individually.**
- ***Ghost writing*** is the use of other person(s) (with, or without payment) to prepare all or part of an item of work submitted for assessment.

Additional Information
Special consideration of assessment*:** If you feel that illness, injury, bereavement or any other critical extenuating circumstance beyond your control has prevented you from completing an item of assessment or affected your performance in that assessment, you may apply for special consideration. Special consideration is not available for items worth less than 10% of the course. Applications for special consideration should be made **within five days** of the due date for the work or examination. In the case of illness or injury, medical consultation should normally have taken place shortly before, or within 24 hours after, the due date for the required work or the date of the test or examination. For details on special consideration, or to make an application, refer to the Examinations Office website http://www.canterbury.ac.nz/exams/. ***You have the right to appeal any decision.

Extensions of deadlines: Where an extension may be granted for an assessment item, this will be decided by application to the course co-ordinator.

Late withdrawal from the course: If you are prevented by extenuating circumstances from completing the course after the final date for withdrawing from the course, you may apply for special consideration for late discontinuation. For details on special consideration, or to make an application, refer to the Examinations Office website http://www.canterbury.ac.nz/exams/. Applications must be submitted ***within five days*** of the end of the main examination period for the semester.

***Missing of tests*:** In rare cases a student will not be able to sit a test. In such cases, the student should consult with the course co-ordinator to arrange alternative procedures. **This must be done well in advance of the set date for the test.**

Past tests and exams: these can be found on our website using the link below:
www.chem.canterbury.ac.nz/for/undergraduate.shtml

***Submission of reports and assignments*: Reports (including lab reports) and assignments should be handed in on time.** Extensions will be granted only in exceptional circumstances (such as illness or bereavement). If an extension is required, as early as possible you should request it from the lecturer concerned.
Note: If you do not submit an assignment for assessment, you will be allotted zero marks, which will affect your final result. You should ensure that you pick up marked assignments and keep them until the end of the course as evidence that the work was completed and marked in the case that either is disputed. To guard against accidental loss, it would be prudent to keep photocopies or electronic copies of anything submitted.

Late Work: Acceptance of late work will be at the discretion of the course coordinator. Please contact the coordinator if your assessment is likely to be late.

Marks and Grades: The following numbers should be considered as a guide to the expected grades under normal circumstances. The School reserves the right to adjust mark/grade conversions, if necessary.

Please note that for all invigilated assessments (tests and exams) worth 33% and above, failure to obtain a mark of at least 40% will result in a final grade no higher than an R at 100 and 200 level, and a C- at 300 level.

Grade:	**A+**	**A**	**A−**	**B+**	**B**	**B−**	**C+**	**C**	**C-**	**D**	**E**
Minimum mark %:	**90**	**85**	**80**	**75**	**70**	**65**	**60**	**55**	**50**	**40**	**0**

Reconsideration of Grades: Students should, in the first instance, speak to the course co-ordinator about their marks. If they cannot reach an agreeable solution, or have questions about their grade in a course, students should then speak to the Director of Undergraduate Studies, Assoc Prof Greg Russell (phone 3694228). Students can appeal any decision made on their final grade. You can apply at the Registry for reconsideration of the final grade within four weeks of the date of publication of final results. Be aware that there are time limits for each step of the appeals process.

Students with Disabilities: Students with disabilities should speak with someone at Equity and Disability Service, phone: 369 3334 (or ext. 93334), email: eds@canterbury.ac.nz).

***Academic Advice*:** Assoc Prof Greg Russell is the coordinator of undergraduate chemistry courses. His interest is in the academic performance and well-being of all such students. Anyone experiencing problems with their chemistry courses or requiring guidance about their B.Sc. in Chemistry should get in contact with Greg.

***Staff-Class Rep Liaison*:** Assoc Prof Greg Russell is in charge of liaison with students in chemistry courses. Your class will appoint a student representative to the liaison committee at the start of the semester. Please feel free to talk to the Academic Liaison or the student rep about any problems or concerns that you might have.

Greg Russell (greg.russell@canterbury.ac.nz, tel. 369 5129)
Director of Undergraduate Studies
School of Physical and Chemical Sciences
2022