

PROD235 Formulation Chemistry

15 points, 0.125 EFTS

General Course Information / Ngā Whakamārama

Occurrences

PROD235-23S1 (C) Semester One 2023

Lectures: Three 50-minute lectures per week.

Tutorials: Tutorials will be scheduled as required and arranged by the Lecturer of each course block.

Details to be confirmed on "My Timetable" and on the web. Any changes to the scheduled times will be communicated by email and/or on LEARN.

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 / Hua Akoranga

By the end of the course you will be able to:

- 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 coloured 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: (9 lectures/3 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: **Ms Anastassiya Lazareva, West 3XX, anastassiya.lazareva@pg.canterbury.ac.nz**

BLOCK 2: (9 lectures/3 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 Preeti Kundu, West 530, preeti.kundu@canterbury.ac.nz**

BLOCK 3: (3 lectures/1 tutorial)

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: **Dr Sarah Kessans, West 325, sarah.kessans@canterbury.ac.nz**

BLOCK 4: (6 lectures/2 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 Sarah Kessans, West 325, sarah.kessans@canterbury.ac.nz**

BLOCK 5: (6 lectures/2 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 Sarah Kessans, West 325, sarah.kessans@canterbury.ac.nz**

BLOCK 6: (3 lectures/1 tutorial)

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: **Ms Anastassiya Lazareva, West 3XX, anastassiya.lazareva@pg.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.

Lecturers / Pūkenga

Course Coordinator, Lecturer

Dr Sarah Kessans, West 325, sarah.kessans@canterbury.ac.nz

Office Hours:

Open door policy. To ensure my availability, email to make an appointment.

Lecturer

Ms Anastassiya Lazareva, West 327,
anastassiya.lazareva@pg.canterbury.ac.nz

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Lecturer

Dr Preeti Kundu, West 530,
preeti.kundu@canterbury.ac.nz

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Assessment / Aromatawai

Test 1: 25%

Test 2: 25%

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.**

Electronic Resources

LEARN: 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.

The use of Artificial Intelligence (AI) bot tools such as **ChatGPT is NOT permitted in this course.** Use of AI bot tools to assist with the generation of any part of your assessments in this course constitutes a breach of instructions and may result in an Academic Misconduct referral. If at all unsure regarding AI bot use, please ask your course coordinator.

Additional Information

Special Consideration applications: If you feel that illness, injury, bereavement or other critical circumstances has prevented you from completing an item of assessment or affected your performance, you should complete a Special Consideration application form, available from the Registry or the Student Health and Counselling Service or online <https://www.canterbury.ac.nz/study/special-consideration/>. This should be within 5 days of the due date for the required work or the date of the 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. You have the right to appeal any decision made, including Special Consideration decisions. For further details on Special Consideration applications, please refer to the weblink above.

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. This will occur only where statistical analysis of marks indicates that the numerical distribution, and subsequently arising grades, is anomalous. Any such adjustments will not be made to the detriment of students' grades.

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

Academic Appeals of Assessments: Students with concerns about assessment processes or grades should be advised to speak first with the relevant lecturer. If the matter cannot be resolved, then the student should meet and discuss the matter with the Head of

Department/School and thereafter follow the procedures outlined in the University procedures <http://www.canterbury.ac.nz/media/documents/postgraduate-/Academic-Appeals-Grievances-Principles-Procedures.pdf> and regulations <https://www.canterbury.ac.nz/regulations/general-regulations/appeals-regulations/>

Students with Disabilities: Students with disabilities should speak with someone at Disability Resource Service (<http://www.canterbury.ac.nz/disability/>, Phone: +64 3 369 3334 or ext 93334, email disabilities@canterbury.ac.nz).

Academic Advice: Head of School, Professor Conan Fee, West 309, phone: +6433694078 or internal Phone: 94078; e-mail: conan.fee@canterbury.ac.nz. His interest is in the academic performance and well-being of all such students. Anyone experiencing problems with their undergraduate product design courses or requiring guidance about their BProdDesign, BProdDesign/BSc or BProdDesign/BCom should get in contact with Conan.

Staff-Class Rep Liaison: Deputy Head of School, Mr Barro de Gast, West 315, phone: +64 3 369 0713 or internal Phone: 90713; e-mail: barro.degast@canterbury.ac.nz. is in charge of liaison with students in product design 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 student rep about any problems or concerns that you might have.