

Molecular Design

Module Information

2022.01, Approved

Summary Information

Module Code	6005APCHEM
Formal Module Title	Molecular Design
Owning School	Pharmacy & Biomolecular Sciences
Career	Undergraduate
Credits	20
Academic level	FHEQ Level 6
Grading Schema	40

Teaching Responsibility

LJMU Schools involved in Delivery
Pharmacy & Biomolecular Sciences

Learning Methods

Learning Method Type	Hours
Lecture	21
Workshop	16

Module Offering(s)

Display Name	Location	Start Month	Duration Number Duration Unit
SEP-CTY	CTY	September	12 Weeks

Aims and Outcomes

Aims	This module will introduce the idea that in order to be useful and valuable, molecules need to have appropriate physical, biological and material properties. By understanding these properties, chemists can design better pharmaceuticals, agrochemicals, cosmetics, consumer products, materials and other chemicals.
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After completing the module the student should be able to:

Learning Outcomes

Code	Number	Description
MLO1	1	Appraise the chemical structure of molecules and relate this to their physical, biological and material properties.
MLO2	2	Formulate and critically evaluate quantitative structure-activity relationships.
MLO3	3	Interpret and qualify the role of QSAR, QM, MM and other modelling techniques in the pharmaceutical, cosmetics and materials industries.

Module Content

Outline Syllabus	<p>The course will begin with the foundations of the area by introducing the very concept of the structure-property relationship and of the QSAR-like approach to modelling this relationship. The applications of this concept to the prediction of physical properties will follow. These two areas will provide sufficient material for students to work in small groups to prepare a poster that will critique a published QSAR model. The final foundation will be an introduction to molecular and quantum mechanics, focusing strictly on their applicability rather than their theoretical underpinnings. The final foundation will be provided by presentations concerning the shape of molecules. These fundamental ideas will then be exemplified for their application to pharmaceuticals, cosmetics and functional materials.</p>
Module Overview	<p>In this module you will be instructed by experts in the School's outstanding research area of computational modelling, particularly applied QSAR. You will be introduced, through cutting edge approaches, to the idea that molecules need to have appropriate physical, biological and material properties to be useful and valuable. By understanding these properties, chemists can design better pharmaceuticals, agrochemicals, cosmetics, consumer products, materials and other chemicals.</p>
Additional Information	<p>This module will be rooted in the School's outstanding research in the area of computational modelling, particularly applied QSAR. Students will be instructed by experts including the latest, cutting edge approaches. The teaching will be a mix of lectures and workshops and will be assessed via a group poster presentation and a final examination. Preparation for the exam will be assisted by sessions using worked examples in all areas that are taught. These will include questions similar to those that will be in the exam and some more challenging examples to help stretch students and build towards the advanced modules in level 7.</p>

Assessments

Assignment Category	Assessment Name	Weight	Exam/Test Length (hours)	Module Learning Outcome Mapping
Report	Report	30	0	MLO1, MLO2, MLO3
Centralised Exam	Examination	70	2	MLO1, MLO2, MLO3

Module Contacts

Module Leader

Contact Name	Applies to all offerings	Offerings
Steven Enoch	Yes	N/A

Partner Module Team

Contact Name	Applies to all offerings	Offerings
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