

Liverpool John Moores University

Title: MOLECULAR DESIGN
Status: Definitive
Code: **6005APCHEM** (121139)
Version Start Date: 01-08-2021

Owning School/Faculty: Pharmacy & Biomolecular Sciences
Teaching School/Faculty: Pharmacy & Biomolecular Sciences

Team	Leader
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Academic Level: FHEQ6
Credit Value: 20
Total Delivered Hours: 39
Total Learning Hours: 200
Private Study: 161

Delivery Options

Course typically offered: Semester 1

Component	Contact Hours
Lecture	21
Workshop	16

Grading Basis: 40 %

Assessment Details

Category	Short Description	Description	Weighting (%)	Exam Duration
Report	Report	Report	30	
Exam	Exam	Exam	70	2

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.

Learning Outcomes

After completing the module the student should be able to:

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

Learning Outcomes of Assessments

The assessment item list is assessed via the learning outcomes listed:

Report	1	2	3
Examination	1	2	3

Outline Syllabus

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.

Learning Activities

Combination of lectures, worked example workshops and poster preparation workshops.

Notes

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.