## **Liverpool** John Moores University

Title: PREDICTIVE TOXICOLOGY

Status: Definitive

Code: **7003APCHEM** (121144)

Version Start Date: 01-08-2021

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

Team	Leader
Steve Enoch	Υ
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Academic Credit Total

Level: FHEQ7 Value: 20 Delivered 40

Hours:

Total Private

Learning 200 Study: 160

**Hours:** 

**Delivery Options** 

Course typically offered: Semester 1

Component	Contact Hours	
Lecture	22	
Workshop	15	

**Grading Basis:** 50 %

#### **Assessment Details**

Category	Short Description	Description	Weighting (%)	Exam Duration
Exam	Exam	Exam	70	3
Report	Report	Workshop report	30	

#### **Aims**

This module aims to outline the principles of how chemistry is used in predictive toxicology. It will cover the chemistry associated with chemical toxicity and how this information can be encoded as computational tools and workflows. It will draw on the physical organic topics taught at earlier levels.

## **Learning Outcomes**

After completing the module the student should be able to:

- 1 Critically appraise the chemistry used in regulatory toxicology to reduce animal usage.
- 2 Formulate chemical mechanisms to demonstrate toxicity and structure-activity relationships.
- 3 Examine and formulate computational tools for use in predictive toxicology.

#### **Learning Outcomes of Assessments**

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

Examination 1 2

Workshop report 2 3

## **Outline Syllabus**

This module will outline how knowledge of chemical mechanisms such as Michael addition can be used to rationalise chemical toxicity that can occur due to exposure to industrial chemicals. The module will cover the regulatory framework governing chemical safety assessment, animal usage and how chemistry is being used to reduce animal testing. The concepts of structure-activity relationships, category formation and the development of computational tools will also be covered. The material will be delivered as a mixture of lectures and workshops during the first semester of the academic year.

# **Learning Activities**

Lectures and workshops

#### **Notes**

The use of chemicals in the modern world is increasingly legislated. Testing of the safety of chemicals is therefore required, but animal testing must be avoided where possible. The use of in silico modelling of chemical toxicity is thus becoming very important, and this is the area covered by this module.