Computational Methods in Toxicology I: Data and Modelling

Module Information

2022.01, Approved

Summary Information

Module Code	7117PHASCI
Formal Module Title	Computational Methods in Toxicology I: Data and Modelling
Owning School	Pharmacy & Biomolecular Sciences
Career	Postgraduate Taught
Credits	20
Academic level	FHEQ Level 7
Grading Schema	50

Teaching Responsibility

LJMU Schools involved in Delivery
Pharmacy & Biomolecular Sciences

Learning Methods

Learning Method Type	Hours
Lecture	16
Practical	12
Workshop	12

Module Offering(s)

Display Name	Location	Start Month	Duration Number Duration Unit
JAN-CTY	CTY	January	12 Weeks

Aims and Outcomes

Aims	To enable students to create and curate chemical datasets, using appropriate quality assessment checks and to use such a dataset to build elementary structure-activity relationship models, cognisant of the principles of good modelling practice.

After completing the module the student should be able to:

Learning Outcomes

Code	Number	Description
MLO1	1	Select appropriate identifiers to ensure the accuracy of chemical structures and discuss key factors in chemical dataset curation.
MLO2	2	Characterise chemicals using appropriate descriptors (physico-chemical properties, fingerprints, metabolic potential) and know how to interpret relevant descriptors
MLO3	3	Develop/interpret elementary structure-activity relationship models (e.g. rules-of-thumb and structural alerts)
MLO4	4	Demonstrate proficiency in the use of a range of computational tools to generate chemical descriptors, assess similarity and rationally group chemicals for the purposes of read-across.

Module Content

Outline Syllabus	Chemical identifiers – advantages/disadvantages of the different typesFinding and curating chemical information, property and activity data; data sources and reliabilityCharacterising chemicals: chemical and biological descriptors and tools / resources for obtaining or predicting values. Hydrophobic, steric, electronic and topological descriptors.Similarity metrics, fingerprints and finding data for “similar” chemicals (including similarity of metabolic profile and metabolite prediction).Relationships between structure and activity (SAR); rules-of-thumb, structural alerts (development and use).Read-across: analogue selection using various similarity metrics; performing, justifying and reporting read-across predictions.Key computational tools and resources associated with the above topics.
Module Overview	
Additional Information	The contents of this module link directly with module 7118PHASCI (Computational Methods II: Advanced Predictive Methods). This module will predominantly be delivered prior to the delivery of 7118PHASCI so that the concepts introduced here can be supplemented and augmented in the following module.

Assessments

Assignment Category	Assessment Name	Weight	Exam/Test Length (hours)	Module Learning Outcome Mapping
Report	Report Structural Alerts	50	0	MLO3, MLO4
Centralised Exam	Exam	50	2	MLO1, MLO2, MLO3

Module Contacts

Module Leader

Contact Name	Applies to all offerings	Offerings
Mark Cronin	Yes	N/A

Partner Module Team

Contact Name	Applies to all offerings	Offerings