Liverpool John Moores University

Title:	COMPUTATIONAL METHODS IN TOXICOLOGY I: DATA AND MODELLING
Status:	Definitive
Code:	**7117PHASCI** (125477)
Version Start Date:	01-08-2021
Owning School/Faculty:	Pharmacy & Biomolecular Sciences
Teaching School/Faculty:	Pharmacy & Biomolecular Sciences

Team	Leader
Mark Cronin	Y
Andrew Leach	
Steve Enoch	
Judith Madden	

Academic Level:	FHEQ7	**Credit Value:**	20	**Total Delivered Hours:**	42
Total Learning Hours:	200	**Private Study:**	158		

Delivery Options
Course typically offered: Semester 2

Component	Contact Hours
Lecture	16
Practical	12
Workshop	12

Grading Basis: 50 %

Assessment Details

Category	Short Description	Description	Weighting (%)	Exam Duration
Report	Alerts	Interim evidence sheet and final report on structural alerts	50	
Exam	Exam	Three from five essay questions	50	2

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.

Learning Outcomes

After completing the module the student should be able to:

1	Select appropriate identifiers to ensure the accuracy of chemical structures and discuss key factors in chemical dataset curation.
2	Characterise chemicals using appropriate descriptors (physico-chemical properties, fingerprints, metabolic potential) and know how to interpret relevant descriptors
3	Develop/interpret elementary structure-activity relationship models (e.g. rules-of-thumb and structural alerts)
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.

Learning Outcomes of Assessments

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

Report Strutural Alerts	3	4	
Exam	1	2	3

Outline Syllabus

Chemical identifiers – advantages/disadvantages of the different types
Finding and curating chemical information, property and activity data; data sources and reliability
Characterising 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.

Learning Activities

Flipped and/or traditional lectures to introduce/cover the topics outlined in the syllabus.
Workshops and hands-on computer-based activities to provide experience of using a wide range of computational methods, particularly in relation to building chemical datasets, developing structural alerts and acquiring data to assist read-across.

Notes

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.