Computational Methods in Toxicology II: Advanced Predictive Methods

Module Information

2022.01, Approved

Summary Information

Module Code	7118PHASCI
Formal Module Title	Computational Methods in Toxicology II: Advanced Predictive Methods
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
Tutorial	2
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 compare the advantages, disadvantages and applications of advanced computational modelling approaches, considering metrics such as adherence to OECD principles, applicability domain, reproducibility, transparency and statistical performance. To equip students with the skills necessary to build, optimise, interpret and report quantitative structure-activity relationship models.

After completing the module the student should be able to:

Learning Outcomes

Code	Number	Description
MLO1	1	Explain the principles of good modelling practice, particularly in relation to OECD principles and published in silico toxicology protocols.
MLO2	2	Critically compare a range of advanced computational methods used in predictive toxicology.
MLO3	3	Interpret existing models and explain the key (statistical) information associated with different types of models
MLO4	4	Build, optimise, explain and report quantitative structure-activity relationship (QSAR) models
MLO5	5	Demonstrate proficiency in the use of a range of computational tools for QSAR model building.

Module Content

Outline Syllabus	Building quantitative structure-activity models, using appropriate software (such as Minitab) with reference to good modelling practice - OECD Principles/ published in silico toxicology protocols.Identifying appropriate endpoint data, descriptors and statistical approaches (e.g. use/interpretation of multilinear regression, r2, rCV2, Q2, outliers, confusion matrices, false positives and negatives, Matthews correlation coefficient, discriminant functions etc.)Pipeline environments for model building; exemplar models (e.g. VEGA; qsardb.org)Interpreting and assessing the usability (for a given purpose) and repeatability of existing QSARs. Model reporting, evaluation and validation: documentation, QSAR model reporting format,Additionally, examples will be provided of more complex variable selection and model building methods – these will be updated according to developments in the area but may include:Genetic algorithms, artificial neural networks, support vector machines, deep learning methodology, random forests etc. Examples of where the methods have been applied, pros and cons of the approaches and comparison of “black box” versus transparent methods in predictive toxicology.
Module Overview	
Additional Information	The contents of this module link directly with module 7117PHASCI (Computational Methods I: Data and modelling). This module will follow logically from the preceding module enabling greater depth of exploration of more complex modelling techniques and state-of-the-art methods. The content will evolve with the latest developments in the area.

Assessments

Assignment Category	Assessment Name	Weight	Exam/Test Length (hours)	Module Learning Outcome Mapping
Portfolio	Portfolio QSAR model	50	0	MLO4, MLO5
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