Liverpool John Moores University

Title:	COMPUTATIONAL METHODS IN TOXICOLOGY II: ADVANCED PREDICTIVE METHODS
Status:	Definitive
Code:	**7118PHASCI** (125478)
Version Start Date:	01-08-2021
Owning School/Faculty:	Pharmacy & Biomolecular Sciences
Teaching School/Faculty:	Pharmacy & Biomolecular Sciences

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Academic Level:	FHEQ7	**Credit Value:**	20	**Total Delivered Hours:**	44
Total Learning Hours:	200	**Private Study:**	156		

Delivery Options
Course typically offered: Semester 2

Component	Contact Hours
Lecture	16
Practical	12
Tutorial	2
Workshop	12

Grading Basis: 50 %

Assessment Details

Category	Short Description	Description	Weighting (%)	Exam Duration
Portfolio	QSAR Model	QSAR evaluation, model building and reporting (QMRF format)	50	
Exam	Exam	Three from five long answer questions	50	2

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.

Learning Outcomes

After completing the module the student should be able to:

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

Learning Outcomes of Assessments

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

Portfolio QSAR model	4	5	
Exam	1	2	3

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.

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, optimising and evaluating quantitative structure-activity relationship models and demonstrating the utility of pipeline environments for model building.

Notes

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.