Computational Approaches at the Chemical-Biological Interface

Module Information

2022.01, Approved

Summary Information

Module Code	7116PHASCI
Formal Module Title	Computational Approaches at the Chemical-Biological Interface
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	24
Practical	2
Tutorial	2
Workshop	12

Module Offering(s)

Display Name	Location	Start Month	Duration Number Duration Unit
SEP-CTY	CTY	September	12 Weeks

Aims and Outcomes

Aims	To introduce students to the building blocks of biological systems (key molecules, organelles and cells), the nature of chemicals (classes/chemical space), structures and properties and how computational approaches are being used to solve contemporary problems at the interface between chemistry and biology.

After completing the module the student should be able to:

Learning Outcomes

Code	Number	Description
MLO1	1	Explain organisation within biological systems including the nature and role of key biological molecules and cell structures.
MLO2	2	Recognise key functional groups in chemistry and demonstrate how structure influences properties of molecules.
MLO3	3	Demonstrate the ability to investigate contemporary issues for which computational methods may provide a solution.
MLO4	4	Formulate and communicate a hypothesis concerning potential applications of computational methods in chemistry and/or biology.

Module Content

Outline Syllabus	Key biological molecules and their function: carbohydrates, lipids, phospholipids, amino acids, proteins, nucleic acids, nucleotides, DNA, RNA, ATP.The cell as the fundamental unit of an organism, building blocks of tissues and organs; basic structure and function of the cell and its key organelles: Cell membranes (phospholipid bilayer, receptors, transporters) ribosomes, nucleus, mitochondria.Processes within the cell and how these can be investigated – genomics, transcriptomics, proteomics and metabolomicsNature of chemicals / functional classes in the context of different types of chemistry (cosmetics, pharmaceutical, agrochemicals).Chemical structures and properties: key functional groups; hydrogen bonding, acid, base theory, pKa, reactivity; electrophiles and nucleophiles; polarizability; shape, volatility, hydrophilicity, lipophilicity, solubility, log P, ionisation, log D (structural features affecting log P/ log D, solubility, acidity). Introduction to computational methods to predict properties of chemicals (e.g. lipophilicity, solubility) and current applications in chemistry and biology.
Module Overview	
Additional Information	This module will serve as a foundation for other modules on the programme ensuring that students who come from a more biologically-based or chemistry-based background will have an appropriate level of knowledge across both disciplines. Formative, diagnostic / self-assessment exercises will be used to identify learning needs of different students, with appropriate support being signposted.

Assessments

Assignment Category	Assessment Name	Weight	Exam/Test Length (hours)	Module Learning Outcome Mapping
Essay	Essay and narrated slides	50	0	MLO3, MLO4
Centralised Exam	Exam	50	2	MLO1, MLO2

Module Contacts

Module Leader

Contact Name	Applies to all offerings	Offerings
Judith Madden	Yes	N/A

Partner Module Team

Contact Name	Applies to all offerings	Offerings