Liverpool John Moores University

Title:	COMPUTATIONAL APPROACHES AT THE CHEMICAL-BIOLOGICAL INTERFACE
Status:	Definitive
Code:	**7116PHASCI** (125476)
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:**	42
Total Learning Hours:	200	**Private Study:**	158		

Delivery Options
Course typically offered: Semester 1

Component	Contact Hours
Lecture	24
Practical	2
Tutorial	2
Workshop	12

Grading Basis: 50 %

Assessment Details

Category	Short Description	Description	Weighting (%)	Exam Duration
Portfolio	Approaches	1500 word essay and 3-5 narrated slides (3 min)	50	
Exam	Exam	Short answer and multiple choice questions	50	2

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.

Learning Outcomes

After completing the module the student should be able to:

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

Learning Outcomes of Assessments

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

Essay and narrated slides	3	4
Exam	1	2

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 metabolomics
Nature 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.

Learning Activities

Flipped and/or traditional lectures to introduce/cover the topics outlined in the syllabus
Workshops aligned with the biology/chemistry syllabus to provide examples or further investigation of key molecules and their features. Practical activity in computer suite using software to obtain and/or predict properties.

Notes

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.