UNIVERSITY of BRADFORD

# Module Descriptor

| Module Details | |
|---|---|
| Module Title | Computational Medicinal Chemistry |
| Module Code | CFS7010-B |
| Academic Year | 2022/3 |
| Credits | 20 |
| School | School of Chemistry and Biosciences |
| FHEQ Level | FHEQ Level 7 |

| Contact Hours | |
|---|---|
| Type | Hours |
| Interactive Learning Objects | 5 |
| Laboratories | 30 |
| Directed Study | 150 |
| Tutorials | 15 |

| Availability | |
|---|---|
| Occurrence | Location / Period |
| BDA | University of Bradford / Semester 2 |

## Module Aims

This module will introduce you to the use of computational chemistry in the drug discovery process. You will develop your skills in building in-silico models of proteins and small molecules in order to predict the affinity of candidate drug compounds to biological targets. You will develop your understanding of how the data that is generated from drug discovery is managed and processed.

## Outline Syllabus

The core methods of computational chemistry, including visualisation techniques, optimisation methods, protein modelling, pharmacophore mapping, QSAR analysis, molecular mechanics, molecular dynamics, perturbation calculations, conformational analysis, ab initio and semi-empirical quantum mechanics.
The role of computational chemistry in designing compounds with biological activity: Modelling drug target structures (mainly proteins but also DNA structures) and building pharmacophores; Designing molecules that fit the pharmacophore; Modelling of binding interactions between small molecules and biological targets using a range of energy calculation methods; The role of molecular flexibility and the environment.

In-silico screening and Quantitative Structure-Activity Relationships (QSAR) to identify drug candidates.

Managing data: Data handling and interpretation: means, SD, t-test; An introduction to bioinformatics; Good logbook keeping.

## Learning Outcomes

| Outcome Number | Description |
|---|---|
| 01 | Explain the key theoretical ideas that underpin the atomistic modelling of biomolecules. |
| 02 | Assess the appropriate computational methods to study particular aspects of biophysics. |
| 03 | Evaluate the results of computational methods in the characterisation of biomolecular systems. |
| 04 | Design computational processes to address a particular research problem. |
| 05 | Interpret data and draw appropriate conclusions. |
| 06 | Evaluate the scientific literature to place computational results in the appropriate context. |
| 07 | Compose the results of computational work into a research report format. |

## Learning, Teaching and Assessment Strategy

The module uses a blended approach to support learning and achievement. Students will enagage with a series of weekly online learning packages. These will include short videos that address key concepts, a set of structured activities (reading, online discissions etc.) that 'scaffold' the learning, and a range of formative tasks that generate feedback on progress. Online workshops and tutorials will also be used to support learing and monitor progress as students move through the curriculum. Practical classes will be held on-campus to provide opportunity to apply knowledge and gain experience using specialist computational packages and techniques. Tutorials will include staff-led demonstration of simulation skills using industry standard software, detailed on-line descriptions of simulation tasks and supervision of students' simulation tasks.
As part of the module, you will be required to complete and report on a mini research project in rational drug design, such as the construction of a protein model structure, the location of the active site in a protein, the pharmacophore mapping of the active site, the design of small molecules fitting the active site or the evaluation of binding affinities of a series of drug candidates using statistical and/or energy calculation tools.

You will receive formative feedback on your laboratory notebooks and your performance in the assigned tasks. During directed study hours, students are expected to undertake reading to consolidate and expand on the content of formal taught sessions, research and prepare for assessments and revise material from formal taught sessions, and to complete the tasks set during the workshops. Your report on the mini research project will be formally assessed.

The VLE will be used to provide access to online resources, lecture notes and external links to websites of interest.

Assessment 1: An oral presentation will cover LOs 1, 2 and 6
Assessment 2: A summative examination will cover LOs 1, 2 and 3
Assessment 3: A report will cover LOs 4, 5, 6, 7

## Mode of Assessment

| Type | Method | Description | Weighting |
|---|---|---|---|
| Summative | Presentation | Oral Presentation (20 minutes) | 25% |
| Summative | Examination - Closed Book | Written examination - Open questions, closed book (1.5 Hrs) | 50% |
| Summative | Laboratory Report | Report for computational experiment 1000 words | 25% |

## Reading List

To access the reading list for this module, please visit https://bradford.rl.talis.com/index.html

*Please note:*
*This module descriptor has been published in advance of the academic year to which it applies. Every effort has been made to ensure that the information is accurate at the time of publication, but minor changes may occur given the interval between publishing and commencement of teaching. Upon commencement of the module, students will receive a handbook with further detail about the module and any changes will be discussed and/or communicated at this point.*

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