UAB

Universitat Autònoma de Barcelona

Degree	Type	Year	Semester
4313473 Bioinformatics	OT	0	1

Contact

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Teachers

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Use of Languages

Principal working language: english (eng)

Prerequisites

To take this module it is necessary to have previously passed both compulsory modules I and II (Programming in Bioinformatics and Core Bioinformatics). Basic notions of Chemistry and/or Biochemistry are also needed.

It is recommended to have the B2 Level in English or equivalent.

Objectives and Contextualisation

The objective of this module is to provide students with knowledge on:

- the physical grounds that sustain molecular modeling

- both the basic and state-of-the-art methods used in the field

- their main fields of application and its limitations

Competences

- Analyse and interpret data deriving from omic technology using biocomputing methods .

- Communicate research results clearly and effectively in English.
- Design and apply scientific methodology in resolving problems.
- Identify the biocomputing needs of research centres and companies in the biotechnology and biomedicine sectors.
- Possess and understand knowledge that provides a basis or opportunity for originality in the development and/or application of ideas, often in a research context.
- Propose biocomputing solutions for problems deriving from omic research.
- Propose innovative and creative solutions in the field of study
- Understand the molecular bases and most common standard experimental techniques in omic research (genomics, transcriptomics, proteomics, metabolomics, interactomics, etc.)
- Use and manage bibliographical information and computer resources in the area of study
- Use operating systems, programs and tools in common use in biocomputing and be able to manage high performance computing platforms, programming languages and biocomputing analysis.

Learning Outcomes

1. Carry out searches (virtual screening) in chemical structures bookshops.
2. Communicate research results clearly and effectively in English.
3. Create models of pharmacophores using the structures of ligand sets.
4. Describe and apply modelling techniques for homology in the three-dimensional protein structure.
5. Describe and characterise computing techniques for molecular dynamics in studying the structure and function of proteins.
6. Describe and classify techniques for predicting the secondary structure using amino acid sequence.
7. Describe the operation, characteristics and limitations of techniques for analysing and visualising protein structures.
8. Design and apply scientific methodology in resolving problems.
9. Establish the corresponding relationships between aminoacidic sequence, three-dimensional structure and proteic function using sources of biological data and the foundations of biocomputing analysis.
10. Identify and apply techniques for CAD, computer assisted drug design
11. Possess and understand knowledge that provides a basis or opportunity for originality in the development and/or application of ideas, often in a research context.
12. Propose innovative and creative solutions in the field of study
13. Recognise and apply different prediction methods of the functions and three-dimensional structure of proteins.
14. Recognise the strategic importance of the protein model in the area of human health, especially in personalised medicine applications and pharmacogenomics.
15. Simulate the union of the ligand and the receptor using ?docking? techniques and molecular dynamics
16. Understand X-ray crystallography and NMR techniques to obtain protein structures
17. Understand the biomolecular and pharmacological techniques used in functional protein assays.
18. Use and manage bibliographical information and computer resources in the area of study
19. Use programs for calculating structure-activity relationships.
20. Use programs for calculating structure.
21. Use programs for visualising structure.

Content

MODULE 4: Structure and Function of Proteins and Drug Design

Part I STRUCTURE CHARACTERIZATION AND MODELLING

Methods for Determining Protein Structure

X-ray Crystallography

NMR

Cryo-electron microscopy

Homology modeling

Part II COMPUTATIONAL CHEMISTRY

Basics in computational chemistry

Energy calculation (PES, QM, Force fields, Hybrid QM/MM)

Conformational Exploration (other than MD: MC, GA, NMA)

Molecular dynamics

Basics

MD in water

MD in the membrane environment

Coarse grain

Scripting & Analysis

Enhanced sampling methods (e.g. US, metadynamics…)

Free energy: TI, FEP, MM/PBSA

Part III DRUG DESIGN

Basics in pharmacology

Hot targets and currently marketed drugs: Kinases, Nuclear receptors, G protein-coupled receptors, Membrane transport proteins

Molecular descriptors

ADME-Tox

Ligand-based and structure-based pharmacophore modelling

Docking

Ligand-protein docking

Protein-protein docking

Virtual screening

MD applications in drug design.

Methodology

The methodology will combine theoretical classes, solving problems in class, practices in the computers lab, seminars and independent study and delivarable tasks. The virtual platform of the UAB will be used.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Seminars	4	0.16	2
Solving problems in class and work in the computing lab	45	1.8	2, 3, 7, 4, 5, 6, 1, 8, 9, 10, 12, 13, 15, 11, 20, 19, 21, 18
Theoretical classes	23	0.92	17, 16, 2, 7, 4, 5, 6, 8, 9, 10, 12, 13, 14, 11, 18
Type: Autonomous			
Regular study	224	8.96	17, 16, 3, 7, 4, 5, 6, 1, 8, 9, 10, 12, 13, 14, 15, 11, 20, 19, 21, 18

Assessment

The evaluation system is organized in two main activities. There will be, in addition, a retake exam. The details of the activities are:

Main evaluation activities

- Student's portfolio (60%): works done and presented by the student all along the course. None of the individual assessment activities will account for more than 50% of the final mark.
- Individual theoretical and practical test (40%): a final exam will take place at the end of this module.

Retake exam

To be eligible for the retake process, the student should have been previously evaluated in a set of activities equaling at least two thirds of the final score of the module. The teacher will inform the procedure and deadlines for the retake process.

Not valuable

The student will be graded as "Not Valuable" if the weight of the evaluation is less than 67% of the final score.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Individual theoretical and practical tests	40%	4	0.16	17, 16, 2, 3, 7, 4, 5, 6, 1, 8, 9, 10, 12, 13, 14, 15, 11, 20, 19, 21, 18
Works done and presented by the student (student's portfolio)	60%	0	0	17, 16, 2, 3, 7, 4, 5, 6, 1, 8, 9, 10, 12, 13, 14, 15, 11, 20, 19, 21, 18

Bibliography

Molecular Modeling principles and applications, A. Leach, Ed. Pearson (i.e. second edition ISBN-13: 978-0582382107)

Essential of Computational Chemistry, C. J. Cramer, (i.e. second Edition, ISBN-13: 978-0470091821)

Introduction to Computational Chemistry. Frank Jensen. JohnWiley § Sons Ltd. (ISBN: 0470011874, 2007)

Python, how to think like a computer scientist http://www.greenteapress.com/thinkpython/

Computational and Visualization techniques for structural bioinformatics using chimera, Forbes J. Burkowski, CRC press