Structure and Function of Proteins and Drug Design 2015/2016

Code: 42398
ECTS Credits: 12

Degree	Type	Year	Semester
4313473 Bioinformatics	OT	0	1

Contact

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Use of languages

Principal working language: english (eng)

Teachers

Leonardo Pardo Carrasco

David Reverter Cendrós

Laura Masgrau Fontanet

Oscar Conchillo Solé

Xavier Daura Ribera

Prerequisites

To carry out this module it is necessary to have passed previously both compulsory modules: Programming in Bioinformatics and Core Bioinformatics. Basic notions in chemistry or biochemistry are also needed.

It is recommended you have a Level B2 of English or equivalent.

Objectives and Contextualisation

The objectives of this module is to provide students with:

- the physical grounds that sustain molecular modeling

- the current state-of-the-art of their implementations

- their main fields of application and limitations

Skills

- 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 the biomolecular and pharmacological techniques used in functional protein assays.
17. Understand X-ray crystallography and NMR techniques to obtain protein structures
18. Use and manage bibliographical information and computer resources in the area of study
19. Use programs for calculating structure.
20. Use programs for calculating structure-activity relationships.
21. Use programs for visualising structure.

Content

Lesson 1. Protein-Strucutre determinataion from crystallographic data

Professor David Reverter

Lesson 2. Basics in Computational Chemistry

Professors Jean Didier Maréchal and Laura Masgrau

Introduction

Quantum chemistry

Molecular mechanics

PES, conformational exploration (no MD)

Multiscale Modeling

QM/MM

Lesson 3. Ligand Based techniques

Professor Leonardo Pardo

Pharmacophore modeling

Similarity search

Lesson 4. Structure based techniques

Professor Leonardo Pardo

Protein ligand Docking

Virtual High-throughput screening

Lesson 5. Homology modeling and fold recognition

Professors Leonardo Pardo and Jean Didier Maréchal

Homology modeling

Loop modeling

Lesson 6. Molecular dynamics

Professors Xavier Daura, Leonardo Pardo and Óscar Conchillo

Basics

Construction of a membrane environment

Protein-protein docking

Lesson 7. Scripting in Structural Bioinformatics

Professor Jean Didier Maréchal

Lesson 8. Applicative fields in Structural Bioinformatics

Professors Jeand Didier Maréchal and Laura Masgrau

ADME

Glycobiology

Lesson 9. Interactomics

Methodology

The methodology will combine theoretical classes, solving problems in class, work in the computing lab, seminars and independent study student. It will use the virtual platform.

Activities

Title	Hours	ECTS	Learning outcomes
Type: Directed			
Seminars	4	0.16	
Solving problems in class and work in the computing lab	45	1.8	
Theoretical classes	23	0.92	
Type: Autonomous			
Regular study	224	8.96	

Evaluation

- Work done and presented by the student (student's portfolio) (60%).
- Individual theoretical and practical tests (40%)

Evaluation activities

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

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)

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