VNIVERSITAT DE VALÈNCIA

Course Guide
44986 Multiscale, machine learning and QSAR methods applied to biomolecules

COURSE DATA

Data Subject	
Code	44986
Name	Multiscale, machine learning and QSAR methods applied to biomolecules
Cycle	Master's degree
ECTS Credits	6.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	Faculty of Chemistry	2	Annual

Subject-matter

Degree	Subject-matter	Character
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	4 - Optativas de segundo	Optional

Coordination

Name	Department
TUÑON GARCIA DE VICUÑA, IGNACIO NILO	315 - Physical Chemistry

SUMMARY

The aim of this course is to provide students with the basic knowledge of machine learning techniques and QSAR (Quantitative Structure-Activity Relationship) methods applied to small and large molecular systems, such as simple reagents or biomolecules. Machine Learning (ML) allows teams to solve problems by learning from data. In recent years ML has been increasingly applied to a wide variety of chemical challenges, from improving computational chemistry to drug and material design and even synthesis planning. This course aims to introduce this rapidly growing reality.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

OUTCOMES

2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should demonstrate self-directed learning skills for continued academic growth.
- Students are able to foster, in academic and professional contexts, technological and scientific progress within a society based on knowledge and respect for: a) fundamental rights and equal opportunities between men and women, b) The principles of equal opportunities and universal accessibility for persons with disabilities, and c) the values of a culture of peace and democratic values.
- Students handle the most common programming techniques in physics and chemistry and are familiar with the essential computational tools in these areas.
- Student are familiar with computational techniques which, based on mechanics and molecular dynamics, are the basis for designing molecules of interest in fields such as pharmacology, petrochemistry, etc.
- Students develop a critical thinking and reasoning and know how to communicate them in an egalitarian and non-sexist way both in oral and written form, in their own language and in a foreign language.
- Students are organized at work demonstrating that they know how to manage their time and resources.
- Students are able to discern between the different existing methods and know how to select the most appropriate method for each problem.

LEARNING OUTCOMES

English version is not available

WORKLOAD

ACTIVITY	Hours	% To be attended
Computer classroom practice	20,00	100
Theory classes	20,00	100
Tutorials	5,00	100
TOTAL	45,00	

TEACHING METHODOLOGY

English version is not available

EVALUATION

Regular assessment

The final mark for the course will be based on: 20% final exam of the course and 80% corresponding to the delivery of a report of exercises proposed by the professor.

Resit

The evaluation will be based on the delivery of a report with the proposed exercises.

REFERENCES

Basic

- Combined Quantum Mechanics/Molecular Mechanics (QM/MM) Methods in Computational Enzymology M.W. van der Kamp and A. J. Mulholland Biochemistry 2013.

  QM/MM Methods for Biomolecular Systems H. M. Senn and W. Thiel (2009), QM/MM Methods for Biomolecular Systems. Angewandte Chemie Int. Ed. 2009.

  A Hybrid Potential Reaction Path and Free Energy Study of the Chorismate Mutase Reaction S. Martí, J. A., V. Moliner, E. Silla, I. Tuñón, J. Bertrán, and M. J. Field Journal of the American Chemical Society 2001.