UAB
Universitat Autònoma de Barcelona

Biomolecular Simulation

Code: 102517
ECTS Credits: 6

2024/2025

Degree	Type	Year
2502444 Chemistry	OT	4

Contact

Name: Jean Didier Pierre Marechal

Email: jeandidier.marechal@uab.cat

Teachers

Maria dels Angels Gonzalez Lafont

Teaching groups languages

You can view this information at the end of this document.

Prerequisites

Chemical Thermodynamics and Kinetics (Fonaments Química 2 i Termodinàmica i Cinètica)

Quantum Chemistry

Previous background in Biochemistry is not essential.

Objectives and Contextualisation

This course has as main objective to introduce students to the basic principles of biomolecular simulations that allow the interpretation at the atomic level of how biological processes take place and of the biomedical and biotechnological applications of biomolecules (drugs, nanoparticles, vaccines...).
Biomolecular simulations are based on the molecular modeling of the biological system or biomolecule of interest.
This modeling involves a series of steps that will be explained in this course both theoretically and in practices, in a balanced equilibrium between concepts, physical equations and on-hands lab:
1) Calculation of the energy of the system as a function of the coordinates (3D structure) of its atoms and molecules by means of Molecular Mechanics and Quantum Mechanics methods;
2) Study of the computational techniques that allow to determine how the energy of the system varies according to its coordinates:
a) Docking techniques;
b) Techniques to minimize the energy;
c) Molecular Dynamics simulations;
d) Methods to calculate free energies.

These different methodologies will be used to study basic biological aspects of biomolecules, as well as in applications for drug design and the study of enzymatic catalysis.

Competences

- "Interpret data obtained by means of experimental measures, including the use of IT tools; identify their meaning and relate the data with appropriate chemistry, physics or biology theories."
- Adapt to new situations.
- Communicate orally and in writing in one's own language.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Manage, analyse and synthesise information.
- Obtain information, including by digital means.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse chemical problems and propose suitable answers or studies to resolve them.
- Resolve problems and make decisions.
- Show an understanding of the basic concepts, principles, theories and facts of the different areas of chemistry.
- Show initiative and an enterprising spirit.
- Show sensitivity for environmental issues.
- Use IT to treat and present information.
- Work in a team and show concern for interpersonal relations at work.

Learning Outcomes

1. Adapt to new situations.
2. Analyse molecular dynamics trajectories.
3. Communicate orally and in writing in one's own language.
4. Determine the structural and energetic changes associated to the pathway of a chemical reaction.
5. Distinguish between the computational methods applied to biomolecules.
6. Learn autonomously.
7. Manage the organisation and planning of tasks.
8. Manage, analyse and synthesise information.
9. Obtain information, including by digital means.
10. Produce simulations of protein-ligand interactions.
11. Propose condensed phase simulations.
12. Propose creative ideas and solutions.
13. Reason in a critical manner
14. Recognise the bases of operating systems and computer language.
15. Resolve problems and make decisions.
16. Show initiative and an enterprising spirit.
17. Show sensitivity for environmental issues.
18. Use IT to treat and present information.
19. Use basic computer simulation.
20. Use the basic methodology of quantum chemistry and molecular mechanics.
21. Visualise biomolecules and certain structural properties by means of display programs.
22. Work in a team and show concern for interpersonal relations at work.

Content

BIOMOLECULAR SIMULATIONS

1. Introduction to molecular modeling of biomolecules.

2. Biomolecules: structure and function. An overview.

3. Molecular mechanics methods for the calculation of the energy.

4. Conformational exploration in biomolecules.

5. Protein-ligand interaction: Docking techniques and drug design.

6. Simulation methods: Molecular Dynamics.

7. Hybrid QM/MM methods for the calculation of the potential energy.

8. Calculations of free energy differences.

9. Enzymatic catalysis: mechanisms and reaction rate.

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Practical sessions	18	0.72	2, 5, 7, 8, 19, 20, 11, 10, 13, 14, 15, 18, 21
Theoretical lectures	34	1.36	2, 4, 5, 19, 20, 11, 10, 14, 21
Type: Supervised			
Tutoring	2	0.08	7, 8
Type: Autonomous			
Bibliographic serach	2	0.08	8, 9
Quizz/Practical reports/Assigned deliverable tasks	14	0.56	1, 2, 6, 3, 16, 4, 5, 7, 8, 19, 20, 17, 9, 11, 10, 12, 13, 14, 15, 22, 18, 21
Study	70	2.8	1, 2, 6, 4, 5, 7, 8, 19, 20, 9, 11, 10, 13, 14, 15

The subject BIOMOLECULAR SIMULATIONS is an optional subject of 6 ECTS belonging to the specialization in BIOLOGICAL CHEMISTRY but it can also be coursed outside this particular specialization.

The teaching methodology of the subject consists on theoretical lecturers in the classroom and practical sessions in the computer room supervised by the professor in charge. Theoretical and practical classes are completed with tutoring hours supervised by teachers in order to resolve doubts. The student must work autonomously on the theoretical contents and the questions posed by the professors in the face-to-face sessions, in the realization of the practices, and in the elaboration of the works of the asignatura that will entail a part of bibliographical research.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Assessment

Continous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Assessment activities	30%	4	0.16	1, 2, 6, 3, 16, 4, 5, 7, 8, 19, 20, 17, 9, 11, 10, 12, 13, 14, 15, 22, 18, 21
Exams	70%	6	0.24	1, 6, 3, 16, 5, 7, 8, 20, 12, 13, 15, 18

The subject has two clearly defined parts (1 and 2) corresponding to the first and second parts of the semester. They will be evaluated independently.

The standard evaluation system for this subject consists of continuous assessment tests with follow-up activities as well as partial exams. Students, if they wish, can request to participate in a single evaluation.

CONTINUOUS ASSESSMENT

In this modality, the weight of each type of activity is as follows:

Exams (70%)

Two partial exams will be conducted on the content of the subject: Partial 1 (P1) (35%) and Partial 2 (P2) (35%).

Follow-up activities (30%)

Throughout the course, two series (S1 and S2) of follow-up activities (quizzes, practical reports, assignments) will be carried out, which will serve as evidence of the student's personal work. These activities are not recoverable.

GRADING

To pass the subject for the course, the following three conditions must be met:

1. Grade for each partial (NP1 and NP2) equal to or higher than 5.0.
2. Final subject grade = 0.70 * (0.50 * (NP1 + NP2)) + 0.30 * (0.50 * (NS1 + NS2)) equal to or higher than 5.0.
3. Attendance to all practical sessions and submission of the report, if required.

If the minimum requirements of 1) and/or 2) are not met, one or both partial exams can be retaken at the end of the course. The grade obtained in the retake will replace the grade obtained in the first attempt.

The completion of practical activities is mandatory.

To participate in the retake, the student must have been previously evaluated in a set of activities whose weight accounts for at least two-thirds of the total grade for the subject. Thus, it is not possible to retake a partial exam that has not been taken.

If the student has been evaluated in a maximum of 25% of the assessments and abandons, the final grade will be NOT EVALUABLE.

UNIQUE ASSESSMENT

Students who have chosen the unique evaluation modality will have to take a final test consisting of an exam on the entire subject matter. The practical activities remain mandatory, and their grades will be considered in the final evaluation.

The unique evaluation test will be held on the same day as the second partial exam for students in the continuous assessment.

The student's grade will be:

Final subject grade = (Grade on the final test * 80 + Grade on practical activities * 20) / 100

Both the grade on the final test and the grade on the practical activities must be equal to or higher than 5.

If the final grade does not reach 5, the student has another opportunity to pass the subject through a recovery exam, which the grade's coordination will schedule. In this exam, 80% of the grade corresponding to the theory part can be recovered. The practical part is not recoverable.

Bibliography

1) Introduction to Computational Chemistry. Frank Jensen. ISBN: 0470011874JohnWiley § Sons Ltd. (2007). (Electronic document availabale at the UAB Library Services)

2) Essentials of Computational Chemistry: Theories and Models. Cristopher J. Cramer. ISBN: 0470091827. JohnWiley § Sons Ltd. (2004). (Electronic and printed documend availabble at the UAB Library Services)

3) Molecular Modelling. Principles and Applications. Andrew R Leach. ISBN: 978-0-582-38210-7. Pearson (2001). (Printed documend availabble from the UAB Library Services)

Software

USCF Chimera

Autodock Vina

CHARMM-GUI (web interface)

Language list

Name	Group	Language	Semester	Turn
(PLAB) Practical laboratories	1	Catalan	first semester	morning-mixed
(TE) Theory	1	Catalan	first semester	morning-mixed