UAB
Universitat Autònoma de Barcelona

Biomolecular Simulation

Code: 102517
ECTS Credits: 6

Degree	Type	Year	Semester
2502444 Chemistry	OT	4	1

Contact

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Use of Languages

Principal working language: catalan (cat)

Some groups entirely in English: No

Some groups entirely in Catalan: Yes

Some groups entirely in Spanish: No

Teachers

Àngels Gonzalez Lafont

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.

Methodology

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.

Activities

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

Assessment

EVALUATION

This subject uses the continuous evaluation to support and assess the learning achievements of the contents and competences by the students.

This continuous assessment will consist of two types of activities: exams and follow-up activities.

Exams (70%)

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

Assessment activities (30%)

Throughout the course, there will be two series (S1 and S2) of follow-up activities (quizzes, practical reports, deliverable tasks) that will serve as evidences of the individual work and learning by the student. These activities do not have a minimum grade required.

QUALIFICATIONS

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

1) Score of each partial exam (NP1 and NP2) equal to or greater than 4,0.

2) Final grade: Final grade = 0.70 * (0.50 * (NP1 + NP2)) + 0.30 * (0.50 * (NS1 + NS2)) equal to or greater than 5.0.

3) Have attended all the practical sessions and delvered the practical report when applicable.

When requirements 1) and 2) are not fulfilled, students can take a second exam for each partial. This second exam can correspond to only one partial exam or to the total contents of the course. The score obtained in these exams will replace that obtained in the corresponding first attempt.

Assisting to the practical sessions is mandatory.

To have the right of being evaluated in these second exams, it is compulsory to have been previously evaluated in a set of evaluation activities whose weight equalsat least two thirds (66.6%) of the total grade ofthe course. Thus, the second exams cannot be taken if any of the partial exams has not been taken first.

If the student has only been evaluated for up to25% of the evaluation activities and abandons the course, the final grade will be NON-EVALUABLE.

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

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)