Universitat Autònoma de Barcelona

2019/2020

Biomolecular Simulation

Code: 102517
ECTS Credits: 6

Degree	Type	Year	Semester
2502444 Chemistry	OT	4	0

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 González Lafont

Prerequisites

Chemical Thermodynamics

Quantum Chemistry

Physical Chemistry

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:
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 ones 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 ones 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. Biomolecules: structure and function.

2. Introduction to molecular modeling of biomolecules.

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.

The teaching methodology of the subject consists of theoretical classes in the classroom given by the lecturer and practical classes in the computer room also directed by the lecturer. These theoretical and practical classes will be completed with tutorizing hours supervised by the lecturer aimed at solving doubts. Moreover, students will have to work on their own on the theoretical contents and questions raised by the lecturer, in the realization of the practical exercises and reports, and in the realization of tasks assigned by the lecturer that will involve a part of bibliographic search.

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 3,5 and the minimum average mark of the two exams is 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.

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.

The second exams can also be taken in order to improve the final mark for the course. In those cases, the new scores will also replace the old ones.

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 equals at 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 to 25% 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).

2) Essentials of Computational Chemistry: Theories and Models. Cristopher J. Cramer. ISBN: 0470091827. JohnWiley § Sons Ltd. (2004).

3) Molecular Modelling. Principles and Applications. Andrew R Leach. ISBN: 978-0-582-38210-7. Pearson (2001).