COURSE: "**BIOPHYSICS SEMINARS**" (2,5 ECTS, Elective)
Classroom: computer room
Coordinator: Dr. Ramon Reigada Sanz (Dep. Química Física, UB)

OBJECTIVES:
In this course, the basic concepts of a wide spectrum of biophysical systems and problems are introduced, and their computational study is addressed. The students will learn different computational techniques, the use of software for molecules visualization and the use of the Protein Data Bank. Neither previous programming skills nor software user expertise are required.

PRACTICAL LESSONS:

1 HOMOLOGY of PROTEINS (Dr. Andreu Alibés, Centre de Regulació Genòmica).
OBJECTIVES: Introduction to the use of the Protein Data Bank, molecular visualization and sequence alignments. Study of different basic modeling strategies and more complex models protein-protein and protein-DNA.

2 STUDY of PROTEIN FLEXIBILITY by COARSE-GRAINED MODELS (Dr. Oliver Carrillo, Parc Científic de Barcelona)
OBJECTIVES: Introduction to 'Brownian Dynamics' (BD) methodology in coarse-grained protein models as an approximation of complete molecular dynamics. Study of the structural properties, elasticity and dynamics of a set of simple proteins.

3 DOCKING applied to DRUG DESIGN (Dr. Jaime Rubio, UB)
OBJECTIVES: Introduction to the Docking technique for drug design. Sampling and scoring of protein-ligand structures. Identification of interactions, ligand optimization, pharmacophores, etc.

4 SIMULATION of the CELL MEMBRANE (Dr. Ramon Reigada, UB).
OBJECTIVES: Coarse-grained Molecular Dynamics simulation of the cell membrane. Study of the self-assembly of amphiphilic compounds in aggregates with a biological interest: bilayers, vesicles, micelles, liposomes, etc.

5 EXCITABLE MEDIA in BIOLOGY (Dr. Blas Echevarría, Dr. Raúl Benítez, UPC)
OBJECTIVES: Study of excitable systems and application to the action potential propagation in neurons and cardiac tissue, and to the propagation of Ca^{2+} waves.

LESSON´S DEVELOPMENT:

- The course will start with a preliminary informative session (2h) that will explain the methodology of the course. The course itself will consist of five practical lessons, each lesson divided in two sessions (in total 2+2 hours).

- During the first session (2h) the professor will introduce the problem under study and its biophysical relevance, the necessary theoretical concepts, the computational approach, and the required software. Some basic examples of use of the software will be suggested under the direct supervision of the professor until the basic computational skills have been achieved.

- During the second session (2h) the student, individually in the computer room, will develop the tasks indicated in the lesson. The professor will assist the students during the session and will also verify that the tasks have been finished correctly.

EVALUATION

- The attendance is compulsory.
- All the students must attend the five sessions and complete the assignments indicated by the professor during the practical session.
- The student must develop, extend and present, as a formal scientific paper, one of the lessons following the indications of the professor.
- The final grade of the course will depend on the quality of the assigned activities, according the judgment of the staff of professors.

In the case that a student misses a lesson, totally or partially, and although well justified, the student will have to present an enlarged written report on all the tasks of the missed lesson.

BIBLIOGRAPHY

- Biophysics of Computation, C. Koch (Oxford University Press, 1999).
- Theoretical Neuroscience, P. Dayan and L. F. Abbott (The MIT Press, 2001).
- Chemoinformatics. Ed. J. Gasteiger and T. Engel (WILEY-VCH, 2003).
- Mechanics of the Cell. D. Boal. (Cambridge University Press, 2002)
- Computational Modeling of Genetic and Biochemical Network. Ed. J.M. Bower and H. Bolouri (MIT Press, 2001)