BIOPHAM Master - Syllabus of the courses proposed at Universitat Politècnica de Catalunya (UPC)

<table>
<tr><td>Course name</td><td colspan="3">MATERIALS SCIENCE OF DRUGS</td></tr>
<tr><td>Credit Points (ECTS)
4</td><td>Workload (Face-to Face)
36h</td><td>Duration
1/3 semester</td><td>Offered (Term)
2</td></tr>
<tr><td>Institution in charge</td><td colspan="3">Universitat Politècnica de Catalunya</td></tr>
<tr><td>Instructors</td><td colspan="3">J. Ll. Tamarit, P. Lloveras</td></tr>
<tr><td rowspan="2">Purpose of the module</td><td>BIOPHAM Track</td><td colspan="2">Mode</td></tr>
<tr><td>1 & 2</td><td colspan="2">Compulsory (all tracks; all options)</td></tr>
<tr><td>Contents</td><td colspan="3">The purpose of this unit is to provide an overview of the thermodynamics of phase equilibrium and phase transitions, with application to the polymorphism of drugs, and to introduce binary phase diagrams and the non-equilibrium glass state, with applications in the field of amorphous drugs.

Course syllabus:

(1) Basic concepts of crystallography: translational order, unit cell, Bravais lattices. Point groups, space groups, crystal systems. Crystallographic planes, reciprocal lattice, Miller indices. From crystal system to molecular structure and geometry: crystals with a base and molecular crystals. Calculation and modelling of diffraction patterns from atomic and structure scattering factors. Solid-state polymorphism of drugs and other organic molecules.

(2) Phase Equilibrium and phase transitions (Thermodynamic Potentials for hydrostatic pvT systems; Maxwell relations; TdS equations; General conditions for equilibrium; Fluctuations; Le Châtelier principle)

(3) Phase transitions and topological pressure-temperature phase diagram (Equilibrium conditions for hydrostatic pvT systems; First-order phase transitions: Clausius-Clapeyron equation. Stability and metastability domains; High-order phase transitions. Group-subgroup phase transitions. Second harmonic generation; Critical and triple points; Topological P-T phase diagram.

(4) Landau theory for phase transitions. Ferroelastic phase transitions. Long-range anisotropic interactions. Self-accommodation. Structural phase transitions. Mechanistic and kinetic classification of phase transitions.</td></tr>
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	(5) Phases out of equilibrium (Glass state and glass transition; dynamics and structural relation in the glass state; pressure dependence of the glass transition temperature; non-equilibrium phases and mesophases of drugs) (6) Binary systems (thermodynamics of mixing, thermodynamic potential; types of binary phase diagrams: eutectic, metatectic and peritectic; solubility and miscibility; metastable and unstable states; nucleation *vs* spinodal decomposition. The course will include laboratory sessions.
Examination	Written midterm exam, problems solved autonomously, laboratory report
Requirement for examination	
More information	CLASSIFICATION: MATERIALS SCIENCE
Learning outcomes	On successful completion of the course students will be able to discuss the equilibrium conditions for a phase or phase coexistence, draw multiphase and/or binary phase diagrams, and distinguish between different equilibrium, metastable, and unstable states, and their relevance for drug formulations.

Course name	BIOPHYSICAL AND MATERIALS SCIENCE CHARACTERIZATION		
Credit Points (ECTS) 4	Workload (Face-to Face) 36h	Duration 1/3 semester	Offered (Term) 2
Institution in charge	Universitat Politècnica de Catalunya		
Instructors	B. Echebarria, T. Pradell		
Purpose of the module	BIOPHAM Track	Mode	
	1 & 2	Compulsory 1B & 2B Optional 1A & 2A	
Contents	The aim of the course is to provide an introduction to chemical physics, especially on liquid solutions (both electrolyte and nonelectrolyte), solid solutions, and homogeneous and hybrid materials, and on the relevant characterization techniques. Course syllabus: (1) Introduction to inorganic chemical physics of electrolyte &		

	nonelectrolyte solutions Types of solutions. Thermodynamics of solutions. Properties of water: The hydrogen bond, solubility of molecules in water, polar and non-polar solvents. Electrical permeability of water. Dissociation: acids and bases, protonation. Properties of solutions: functional groups, hydrophilic and hydrophobic interactions; solubility; diffusion. Colligative properties: boiling-point elevation, freezing point depression, osmotic pressure. Surface tension, capillarity. Water phase diagram and anomalies; aqueous electrolytes; non-electrolyte solutions. Electrostatics of salty solutions: biopolymers (polyelectrolytes) and biomembranes in water; Poisson-Boltzmann equation, Debye-Hückel model, electric double layers, ion and proton conduction; transport properties. (2) Introduction to materials science properties Cohesive interactions; structural and mechanical properties of homogeneous solids; organic molecular solids; non-miscible systems: morphology and properties of phase-separated materials (3) Laboratory techniques - Elemental analysis: photoelectron & mass spectroscopy (XPS, UPS, Auger, secondary ion mass spectroscopy) - Chemical analysis: optical and vibrational spectroscopy (UV-vis, IR, Raman), nuclear magnetic resonance (NMR) - Morphological analysis: contact angle, powder X-ray diffraction (XRD), tomography (microCT), NMR-imaging, electron microscopy (SEM, TEM, energy loss/secondary electron spectroscopy) - Phase-change analysis - Mechanical, electrical and optical characterization - A pharmaceutical application: optical measurement of the dissolution kinetics and solubility of a drug (4) Applications to pharmaceutics, drug formulation, & biophysical pharmacology: - Experimental techniques for electrolyte and non-electrolyte solutions - Small Molecules (drugs): HPLC, Chromatography, Mass spectroscopy, ICP-MS - Characterization of Nanoparticles: Molecular sizes (Dynamics light scattering, DLS), Surface charge (zeta potential, with conductivity measures) - Characterization of Biomolecules: chromatography, gel electrophoresis, Western Blot. Proteomics
Examination	Report on a case study, handed-in solved problems, midterm/final exam
Requirement for examination	

More information	CLASSIFICATION: BIOPHYSICS/MATERIALS SCIENCE
Learning outcomes	On successful completion of the course students will be able to: ● Understand and describe the fundamental properties of aqueous solutions and complex materials ● Describe the application of experimental physicochemical methods to the solid and liquid states, and choose the appropriate experimental techniques that serve a specific purpose

Course name	STOCHASTIC METHODS FOR OPTIMIZATION AND SIMULATION		
Credit Points (ECTS) 4	Workload (Face-to Face) 36h	Duration 1/3 semester	Offered (Term) 2
Institution in charge	Universitat Politècnica de Catalunya		
Instructors	J. Casulleras, G. Astrakharchik		
Purpose of the module	BIOPHAM Track	Mode	
	1 & 2	Optional (recommended for tracks 1A, 2A)	
Contents	This course will give students an operative knowledge of computational simulation and optimization techniques based on stochastic methods. Course syllabus: (1) Monte-Carlo Integration. Sampling techniques and variance reduction. (2) Stochastic optimization: simulated annealing and genetic algorithms. (3) Dynamic Monte Carlo: random walks and the diffusion equation. (4) Classical Monte Carlo simulations: from simple to molecular systems and biomolecules. (5) Application of Monte Carlo methods to quantum systems.		
Examination	The final mark for this course is computed as 0.4 a + 0.4 b + 0.2 c, where a is the mean grade of each practical homework, b is the grade of the final project and c is the rating of written questions concerning the final project.		
Requirement for examination			
More information	CLASSIFICATION: COMPUTATIONAL PHYSICS		

Learning outcomes	Learning outcomes: on successful completion of the course students will be able to: - Devise efficient sampling methods for sampling any multi-dimensional probability distribution. - Make use of stochastic methods for the optimization of complex problems with arbitrary model-functions. - Perform Monte Carlo simulations of both classical and quantum systems.

Course name	LARGE FACILITIES: SYNCHROTRON AND NEUTRON SOURCES		
Credit Points (ECTS) 5	Workload (Face-to Face) 45h	Duration 1/3 semester	Offered (Term) 2
Institution in charge	Universitat Politècnica de Catalunya		
Instructors	P. Bruna, Y. A. Koubychine, L. C. Pardo		
Purpose of the module	BIOPHAM Track	Mode	
	1 & 2	Compulsory (all tracks; all options)	
Contents	The purpose of this unit is to learn the basics of facilities such as synchrotrons and spallation sources, and the kind of characterisation techniques that they allow. Program: (1) Particle accelerators, synchrotron radiation and neutron sources. (Basics of particle accelerators: general introduction, types of accelerators, methods of acceleration; circular accelerators, magnetic systems; main accelerator systems: RF, diagnostics; Beam characteristics. Generation of e.m. radiation: Bremsstrahlung, synchrotron radiation, characteristics and generation, insertion devices; beamlines and experiments: the Alba synchrotron; ion accelerators; spallation sources. (2) Data analysis and elementary scattering theory (Frequentist data analysis; data and errors: a statistical view; classical fitting methods; statistical distributions; hypothesis testing; Bayesian data analysis: bayesian statistics and probability distribution functions; Bayes theorem, measurement, fitting functions; Marcov Chain Montecarlo method; Model selection in Bayesian statistics; basics of X-ray and neutron scattering (Bragg Law; the phase problem; reflectometry and small angle scattering; diffraction of liquids and amorphous materials; inelastic scattering: coherent and incoherent scattering, Van –Hoff functions. (3) Some synchrotron and Neutron applications (XRD and powder diffraction; EXAFS – XANES; hard X-ray synchrotron imaging Techniques; Neutron applications: inelastic neutrons scattering methods: Time of flight, Spin Echo, Backscattering; magnetism using neutrons; imaging		

	using neutrons; speciallized seminars by ALBA staff; practices at ALBA in the accelerators group: magnetic measurements, RF measurements, vacuum system
Examination	The evaluation will consist of a mark for small homework projects and exercises of each module (25%), and one for the final project (75%). The latter will consist of two marks, one for the written report and one for the oral presentation.
Requirement for examination	
More information	CLASSIFICATION: ENGINEERING/MATERIALS SCIENCE
Learning outcomes	On successful completion of the course students will be able to: ● Explain the basic functioning of a synchrotron radiation source and a spallation source, as well as the different properties that synchrotron light or neutrons can possess and how they can be tuned ● Describe how synchrotron light and neutrons can be used to investigate condensed matter, how collected data should be analysed, and what information can be extracted from the data ● Identify the advantages of using a large facility to perform experiments, and the most suitable technique to tackle a given experimental problem

Course name	MOLECULAR AND SOFT CONDENSED MATTER		
Credit Points (ECTS) 4	Workload (Face-to Face) 36h	Duration 1/3 semester	Offered (Term) 2
Institution in charge	Universitat Politècnica de Catalunya		
Instructors	R. Macovez, C. Alemán		
Purpose of the module	BIOPHAM Track	Mode	
	1 & 2	Compulsory (all tracks; all options)	
Contents	This unit introduces the physics of molecular and macromolecular condensed phases such as liquids, glasses, liquid crystals, plastic and orientationally disordered crystals, polymers and polymer gels. Course syllabus: (1) Basics of molecular condensed matter: introduction (polymorphism, glasses, complex fluids: mesophases & polymers); classification and mechanism of phase transitions (first order,		

	continuous, glassy; nucleation and growth); van der Waals theory; microscopic constituents, effective interactions, disorder & dynamics; experimental tools & linear response theory; Boltzmann distribution and partition function (2) Single component systems: structural glasses, primary and secondary relaxations, aged and stable glasses; orientationally disordered solids and plastic crystals; amorphous and semicrystalline linear polymers; rotational isomeric state model; ideal chains and entanglement, normal and segmental relaxations; viscoelasticity; polymers networks, gelation and rubber elasticity; conjugated and conductive polymers; thermotropic liquid crystals and liquid crystal polymers) (3) Introduction to binary systems and binary equilibrium and non-equilibrium phase diagrams: heterointeractions; glass-forming mixtures; binary plastic crystals; polymer blends, solutions, and dispersions; block copolymers; polymer gels and hydrogels, swelling; superhydrophobic, superhydrophilic/olephobic, superamphiphilic, and self-healing polymer coatings. Self-assembly in condensed matter: biopolymers, helix-coil & coil-globule transitions; surfactant-water systems, biomembranes, lyotropic liquid crystals, emulsions; semiflexible polymers & cytoskeleton; colloidal systems (glasses, crystals, nematics, gels); Applications to drug encapsulation, controlled drug release, and drug delivery.
Examination	Oral and written presentation of case study (60%), written midterm exam (40%)
Requirement for examination	
More information	CLASSIFICATION: MATERIALS SCIENCE
Learning outcomes	On successful completion of the course students will be able to: • describe the phases of single-component molecular systems, and the main experimental techniques available to study molecular dynamics and phase transitions • discuss the (dynamic) disorder present in a phase and its impact on rheological/mechanical properties and on vitrification • describe the main theories that describe the properties of glasses, liquid crystals, linear polymers and polymer networks, as well as their main technological applications

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<table>
<tr><td>Course name</td><td colspan="3">COMPLEXITY IN BIOLOGICAL SYSTEMS</td></tr>
<tr><td>Credit Points (ECTS)
4</td><td>Workload (Face-to Face)
36h</td><td>Duration
1/3 semester</td><td>Offered (Term)
2</td></tr>
<tr><td>Institution in charge</td><td colspan="3">Universitat Politècnica de Catalunya</td></tr>
<tr><td>Instructors</td><td colspan="3">S. Alonso, A. Pons</td></tr>
<tr><td rowspan="2">Purpose of the module</td><td>BIOPHAM Track</td><td colspan="2">Mode</td></tr>
<tr><td>1 & 2</td><td colspan="2">Optional (recommended for tracks 1B, 2B)</td></tr>
<tr><td>Contents</td><td colspan="3">Course syllabus:
(1) Biological networks (examples in system biology: metabolic networks, interactome, regulatory and signalling networks; biological neural networks; networks in ecology and epidemiology
(2) Complex spatio-temporal dynamics in biology (oscilations, excitability, bistability; sinchronization in biological systems: neural networks; spatio-temporal chaos: cardiac fibrillation
(3) Analysis of complex biosignals (deterministic and stochastic signals; statistical properties; non-lineal time-series analysis of series temporalis)
(4) Self-organization in biological systems (morphogenesis; self-assembly: protein folding, membrane formation); growth processes: chemotaxis, tumour growth)
(5) Collective motion and active matter (flocking, swarming and herd; cell migration)</td></tr>
<tr><td>Examination</td><td colspan="3">The final mark for this course will be as follows mark = W*0.5 + O*0.5, where W is the total mark of written examinations, which will include a written exam, applied activities, case studies or problem resolution, and O is the total mark of oral examination, consisting of an oral exam or oral presentation</td></tr>
<tr><td>Requirement for examination</td><td colspan="3"></td></tr>
<tr><td>More information</td><td colspan="3">CLASSIFICATION: BIOPHYSICS</td></tr>
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Learning outcomes	On successful completion of the course students will • have a basic knowledge of some biological phenomena (from the molecular or cellular level to the macroscopic level), and understand what a complex system is and how to characterize it • be able to employ numerical techniques as well as a software specific to the course • be able to employ theoretical/practical knowledge to solve problems of biological interest and present the results in a broader context, using the appropriate terminology

Course name	MACHINE LEARNING WITH NEURAL NETWORKS		
Credit Points (ECTS) 4	Workload (Face-to Face) 36h	Duration 1/3 semester	Offered (Term) 2
Institution in charge	Universitat Politècnica de Catalunya		
Instructors	E. Romero, J. Delgado		
Purpose of the module	BIOPHAM Track	Mode	
	1 & 2	Optional (all tracks; all options)	
Contents	Course syllabus: (1) Introduction to Machine Learning (fundamental problem and its inherent complexity; general approaches for its solution) (2) Classic Neural Networks models (Hopfield model; recurrent Boltzmann Machines (BM) and Restricted Boltzmann Machines (RBM); learning with BM y RBM: gradient descent, Contrastive Divergence and its variants; single-layer perceptrons (SLP): lineal and logistic regression, Rosenblat perceptron; multi-layer perceptrons (MLP): learning with MLP, back-propagation; Convolutional Neural Networks (CNN): model, link to MLP, and learning) (3) Deep Learning: link with classical models and modern learning techniques.		
Examination	The final mark for this course is computed as 0.2*M_1 + 0.2*M_2 + 0.6*M_3, where M_n is the grade of each practical homework. For the latter, the students will be provided with a code structure, and they will have to implement specific functions and run virtual experiments in which different machine learning strategies will be employed.		
Requirement for examination			

More information	CLASSIFICATION: ENGINEERING
Learning outcomes	On successful completion of the course students will be able to: - State the fundamental problem and complexity of Machine Learning, and acquire a global view of the different Machine Learning techniques; - Understand and explain classical models of Neural Networks such as the Hopfield networks, Boltzmann Machines, Single- and Multi-layer Perceptrons, and Convolutional networks. - Implement the standard training techniques in these models, and put them in relation with the issue of the Deep Learning and its solution techniques.

Course name	SHORT INTERNSHIP (Introduction to research projects)		
Credit Points (ECTS) 5	Workload (Face-to Face)	Duration 1/3 semester	Offered (Term) 2
Institution in charge	Universitat Politècnica de Catalunya		
Instructors	Supervisor from Institute/Company + Tutor from UPC		
Purpose of the module	BIOPHAM Track	Mode	
	1 & 2	Compulsory (all tracks; all options)	
Contents	Research/industrial internship		
Examination	Evaluation by Supervisor. Written report evaluated by Tutor.		
Requirement for examination			
More information	CLASSIFICATION: dependent on project The internship should last 1 or 2 months, and take place **in one of the EU countries** in academic or industry laboratory, large scale research facility or computer center. EU countries: Austria, Belgium, Bulgaria, Croatia, Republic of Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Poland, Portugal, Romania, Slovakia, Slovenia, Spain and Sweden.		

Learning outcomes	After completion of the internship, the students will have hands-on, operative knowledge of a research project carried out either at a university, research institute or facility, or private company. They will actively participate in a line of research or development of a product, and become acquainted with the work environment which is the target of the Erasmus Mundus programme.

Course name	ROSETTA STONE LANGUAGE COURSE		
Credit Points (ECTS) 4	Workload (with computer programme) 24 h	Duration 1/2 semester	Offered (Term) 2
Institution in charge	Universitat Politècnica de Catalunya (through the Universitat de Barcelona)		
Instructors			
Purpose of the module	BIOPHAM Track	Mode	
	1 & 2	Compulsory (all tracks; all options)	
Contents	One level (A1, A2, B1, B2, C1) of a foreign language		
Examination	Online written and oral exercises		
Requirement for examination			
More information	CLASSIFICATION: LANGUAGE COURSE		
Learning outcomes	During this course, the students carry out excercises and practice a foreing language either : - toward the C1 level of proficiency in English - toward learning basic notions of grammar, vocabulary and phraseology in another European language (level A1 or higher depending on the student's initial skills).		

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Legend of BIOPHAM Tracks & Options:

1A= Track 1: Soft Matter & Biopharmaceuticals; Option A: Modelling & Simulation

1B= Track 1: Soft Matter & Biopharmaceuticals; Option B: Advanced experimental techniques

2A= Track 2: Condensed-matter & pharmaceuticals; Option A: Modelling & Simulation

2B= Track 2: Condensed-matter & pharmaceuticals; Option B: Advanced experimental techniques