General Information	MASTER DEGREE IN BIOTECHNOLOGIES
Title of the subject	DRUG DESIGN AND DEVELOPMENT
Degree Course (class)	Industrial and Environmental Biotechnology (LM-8)
ECTS credits	6
Compulsory attendance	yes
Language	italian
Academic year	2020-2021

Subject Teacher		
Name and Surname	Orazio Nicolotti	
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Place and time of reception	by email	
ECTS credits details	Discipline sector (SSD)	Area
	CHIM/08	Chemistry

Study plan schedule	Year of study plan	Semester
	II	I

Time management	Lessons	Laboratory	Exercises	Total
CFU	5	1		6
Total hours	125	25		150
In-class study hours	40	12		52
Out-of-class study hours	85	13		98

Syllabus	
Prerequisites / Requirements	
Expected learning outcomes (according to Dublin descriptors)	
Knowledge and understanding	Learning about main methods for the design of molecules of pharmacological or diagnostic interest.
Applying knowledge	Use of specific methodologies and technological platforms (molecular modeling) for the identification of molecular targets of biotechnological interest.
Making informed judgments and choices	Informed evaluation and interpretation of experimental data.
Communicating knowledge	Skills to analyze, propose and critically discuss the data with general audience.

Capacities to continue learning	Critical approach to the medicinal chemistry topics.
Study Program	
Content	Fundamental interactions between molecules. Van der Waals forces. Hydrophobic effect. Ionic interactions. Dipolar interactions. 1D, 2D and 3D molecular descriptors. Quantitative Structure-Activity / Property Relationship. 1D, 2D and 3D molecular representation. Database searching. Similarity and molecular diversity. Principal component analysis, cluster analysis, genetic algorithms, multi-objective optimization techniques. Experimental design. Applicability domani. Basic of predictive toxicology. Pharmacophore models. QSAR models. Hansch equation. Free-Wilson equation. Craig Plot, CoMFA, GRID. Molecular mechanics. Conformational Analysis. Three-dimensional structure of proteins and active site. Protein Data Bank, Protein-Molecule Interaction, Molecular Docking. Molecular dynamics. De novo design. Virtual screening.
Bibliography and textbooks	• R. Leach, Molecular Modelling: Principles and Applications, Pearson Education EMA • Graham L. Patrick; Introduzione alla Chimica farmaceutica (EdiSES) • Gasco, Gualtieri, Melchiorre: Chimica Farmaceutica (Casa Editrice Ambrosiana)
Notes to textbooks	
Teaching methods	
Assessment methods (oral, written, ongoing assessment)	
Evaluation criteria (describe criteria for each of the above expected outcomes)	Knowledge of the basic methods for the design of molecules of pharmacological or diagnostic interest. Use of programs for molecular modeling. Critical evaluation of experimental results.
Further information	