

General Information	MASTER DEGREE IN BIOTECHNOLOGIES		
Title of the subject	Molecular Modeling and Protein engineering		
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	Ciro Leonardo Pierri	
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Place and time of reception	0805443614	
ECTS credits details	Discipline sector (SSD)	Area
	Bio/10	---

Study plan schedule	Year of study plan		Semester	
	2020/2021		1st	
Time management	Lessons	Laboratory	Exercises	Total
CFU	5	1		6
Ore totali	125	25		150
Ore di didattica assistita	40	12		52
Ore di studio individuale	85	13		98

Syllabus	
Prerequisites / Requirements	Knowledge of unix like OS and scripting languages (python, perl, bash)
Expected learning outcomes (according to Dublin descriptors)	
Knowledge and understanding	Solving problems related to protein engineering and functional characterization
Applying knowledge	Several software for dealing with protein sequences and protein structural data
Making informed judgments and choices	Students will learn to create the right context for solving a biological problem by using existing data about protein sequences and structures.
Communicating knowledge	Students will learn to transfer the acquired high-tech knowledge based on the employment of advanced molecular modeling tools to colleagues that need those technology and are not able to deal with it. They will also learn to coordinate the activities of a working group

	for planning and validating the computational analyses necessary for finding a solution to a biological problem.
Capacities to continue learning	The acquired know-how will represent the basis for creating the right context for most of biological problems concerning the characterization of a protein of unknown function within a metabolic pathway.
Study Program	
Content	Introduction to molecular modeling and protein engineering; Sequence databases and tools (blast, biomart) for sequence sampling; text editors (TextPad; Gedit; TextWrangler); sequence editors (Jalview, Bioedit) and sequence comparative analyses; molecular visualizers (SPDBV, PyMOL, Chimera, Autodock); tools for secondary structure prediction and folding recognition methods (psipred, pgenthreader and itasser); tools for manual interactive comparative modeling and in silico mutagenesis (SPDBV and Modeller); tools for docking analyses and virtual screening (SwissDock, Autodock)
Bibliography and textbooks	Lehninger Principles of Biochemistry; Textbook of structural biology; DeepView Manual https://spdbv.vital-it.ch/manual_guide.html ; Autodock tutorials http://autodock.scripps.edu/fags-help/tutorial ;
Notes to textbooks	The discussed slides are available for all the attendees
Teaching methods	Talk, round tables, PC simulation
Assessment methods (oral, written, ongoing assessment)	Oral presentation of the proper own project about protein functional characterization developed along the course
Evaluation criteria (describe criteria for each of the above expected outcomes)	Students have to show the acquired skills in planning a project for answering a biological problem concerning the involvement of a protein of unknown function/structure by using computational approaches. Students have also to show their abilities in evaluating results of their computational analyses/predictions and to plan their validation in <i>in vitro/in vivo</i> assays. For showing the acquired skills the attendees will prepare a report in the form of a scientific paper to be discussed by preparing a ppt presentation.
Further information	