MASTER IN BIOINFORMATICS (2023-2024)
M1 ISDD Research Course:
Design of bioactive molecules (French diploma or double Franco-Italian diploma)

SEMESTER S1 UNIVERSITY of STRASBOURG (30 ECTS)

UE1 METHODOLOGY (10 ECTS)
Coordinators: G. MARCOU , DALBAVIA JO, GIUSEPPONE N.

Title: Methodology

Teaching coordinators: G. Marcou, JO Dalbavie, N. Giuseppone

Programme: Operating systems and networks

Components and peripherals of a PC. The DOS/Windows7/Linux environment. Administration. Principles of operating systems. Command interfaces and automation scripts. Local networks, TCP/IP. Shell scripts: the bash

Targeted skills:

Disassembly/reassembly of material. System installation. Networks Security Write and execute a script

Programme: Statistical methods

Descriptive statistics, Statistical tests, One-Way ANOVA, Single and multiple regression, Stepwise regression, Principal Component Analysis, Advanced methods: Partial Least Square (PLS) and Logistic Regression.

Targeted skills:

Implementation in specific cases for chemistry. Use of EXCEL for statistical analysis.

Programme: Organic chemistry

General information on organic compounds Liaisons, conformations, stereochemistry. Reactions and reaction mechanisms. Alkanes, alkenes, alkynes and cyclic hydrocarbons. Halogenated derivatives. Alcohols, epoxides, ether oxides, thiols, thioethers, amines. Aldehydes, ketones, carboxylic acids and derivatives. Arenes.

UE2 MOLECULAR MODELLING (8 ECTS)
Coordinator: R. SCHURHAMMER

Title: Molecular Modelling

Teaching coordinator: R. Schurhammer

Programme: Molecular Modelling

Introduce three complementary approaches to the modelling of molecular architectures: database investigations, construction and minimisation by force field methods, and quantum mechanics.

Targeted skills:

Force field methods. Use of structural databases. Overview of quantum chemistry methods.

Programme: Modelling practical

Modelling of structure and properties of organic molecules (quantum chemistry, mechanics and molecular dynamics, chemoinformatics). Modelling software.

Targeted skills:
Conformational sampling. Theoretical calculations of molecules parameters. Structural research in the CCDC database.

Programme: Introduction to Therapeutic Chemistry
Knowledge and objectives shared by chemists, phytochemists and biologists regarding active substances. Chemical nature and origin of active substances. Physico-chemical properties and metabolisation of active substances. Production. Control. The world of medicine.
Targeted skills:
Strategies and methods for identifying and optimising active substances. Pharmaceutical industry and R & D.

UE3 CHEMOINFORMATICS (10 ECTS)
Coordinator: A. VARNEK

Title: Chemoinformatics

Teaching coordinator: A. Varnek

Programme I:
Representation of structures by computer (1D, 2D, 3D). Elements of graph theory. SMILES and InChi chains. Molecular imprints. Pharmacophores. MOL, SDF, RXN and RDF formats. Structural and substructural research. Conformational analysis. Similarity and diversity of molecules.

Targeted skills:
Create/manage chemical data using commercial software. Processing, creation of chemical data.

Programme II:
Molecular descriptors (1D, 2D, 3D). Structure-activity methods (QSAR/QSPR). QSAR in 3D: comparative analysis of molecular fields ("CoMFA"). Virtual screening and *in silico* design of new compounds. Filters. Docking.
Targeted skills:
Be able to select relevant descriptors, obtain QSAR models and use them for virtual screening.

Programme: *In silico* Chemical Diversity
Chemical database. Similarity and diversity of molecules. Chemical space. Clustering methods. Preparation of various data sets. Generation of combinatorial chemo libraries Targeted skills:
Create and manage a chemical database. To qualitatively analyse the content. Suggest "new" compounds.

UE4 COMMUNICATION (2 ECTS)
Coordinator:

Title: Communication

Teaching coordinator:

Programme: Disciplinary English
Intensive English course at the beginning of the semester supported by lectures and homework in English. Understanding, expression, pronunciation. + Guided English self-study where students use resources on the Internet or resources installed on computers**.**

Targeted skills:
Understand articles and lectures in English. Mastery of the meaning of words used. Intelligible pronunciation.

Programme: Conferences
Lecture cycles given by renowned researchers and industrialists. Examples: Artem Cherkasov (Vancouver, Canada), Alexander Tropsha (Chapel Hill, USA), Joao Aires de Susa (Lisbon), Markus Gastreich (Biosolvit), Philippe Vayer (Servier).

Targeted skills:
Have an objective look at the state of knowledge in Chemoinformatics and Drug Design.

Programme: Presentation of articles
Bibliographic work and article analysis

SEMESTER S2 UNIVERSITY DEGLI STUDI DI MILANO (30 ECTS)

UE1 PROGRAMMING IN C (6 ECTS)
Coordinator: C. LORENZO

Title: Programming in C
Teaching coordinator: C. Lorenzo
Programme:
Basic aspect of C programming. Language for numerical analysis and statistics purposes.
Generalities about programming languages. Source files and executable files. Compilers. Variable types. Input-output operations. While and for loops. Conditional constructs. Pointers. Array manipulation. String manipulation.

Targeted skills:
To be able to write and execute simple codes in C

UE2 STRUCTURAL BIOLOGY AND ENZYMOLOGY (6 ECTS)
Coordinator: MR VANONI

Title: Structural Biology and Enzymology

Teaching coordinator: Mr Vanoni

Programme:
Structural Biology and Enzymology Introduction to the identification of biological drug targets by bioinformatic, genomic, transcriptomic, and proteomic techniques. Criteria for the validation of pharmacological targets. Molecular recognition and nature of ligand binding sites. Structure-function
Synthetic Techniques Applied to the Design and Synthesis of Biologically Active Principles Expanded role of chemistry in all phases spanning the initial concept idea, the rational design, the synthesis, and the structural optimisation of a pharmacologically active molecule.

Targeted skills:
Structural biology and enzymology in structural design, synthesis and structural optimisation of a pharmacologically active molecule.

UE3 MEDICINAL CHEMISTRY (6 ECTS)
Coordinator: L. BELVISI

Title: Medicinal chemistry

Teaching coordinator: L. Belvisi

Programme:
Principal phases of drug action. Pharmacokinetics: Absorption, Distribution, Metabolism, and Excretion of drugs. Pharmacodynamics: the molecular targets of drugs and the receptor concept. Principal phases of drug discovery and development process. LEAD identification.

Targeted skills:
Knowledge on Principal phases of drug action

UE4 SIMULATION, MODELLING AND BIOMOLECULES (6 ECTS)
Coordinator: S. PIERACCINI

Title: Simulation, Modelling and Biomolecules

Teaching coordinator: S. Pieraccini

Programme:
Molecular mechanics principles. The concept of atom type. Force fields functional form. Molecular dynamics. Integration of Newton equations. Periodic boundary conditions. Calculation of non bonded terms. Setup of an MD simulation. The sampling problem. Application to the protein folding problem

Targeted skills:
Molecular modelling for Biomolecules, molecular dynamics, and sampling simulation

UE5 BIOACTIVE MOLECULES (6 ECTS)
Coordinator: L. BELVISI

EC 501 Synthetic methods in Biotechnology or CHIM06 courses (6 ECTS) (
Or
Bioinformatics & language (6 ECTS) (if Erasmus semester French degree)
Coordinator: L. BELVISI