MASTER BIOINFORMATIQUE
Program EM Chemoinformatics+ 2024-2025 :
In Silico Drug Design – Bioactive Molecules MSc
Paris Cité – Degli studi di Milano
(double diplôme franco-italien)

SEMESTRE 1 - Université Paris Cité (30 ECTS)

UE1	**Methodology (A Badel, 10 ECTS)** **BQAAY000** Initiation to Unix and R (G. Moroy) **BQ2AY040** Mathematics I- Forcefield method/physical chemistry (A-C. Camproux & S. Pasquali) (3 ECTS) **BQAAY070** Python programming1 or **BQAAY080** Python programming2 (P. Fuchs & P. Poulain) (3 ECTS) **BQAAY020** Statistics and R (L. Regad) (3 ECTS) **BQ2AU150** English communication (1 ECTS)
UE2	**Chemistry (O Taboureau, 12 ECTS)** **BM0BY250** RéSO: Reactivity and organic synthesis (F. Chau) (3 ECTS) **XXX** Biological Chemistry (O. Reinaud) (3 ECTS) **BQ2AE170** Chirality - non covalente bounds (F. Maurel, O. Taboureau) (3 ECTS) **XXX** NMR for molecules (N. Giraud) (3 ECTS)
UE3	**Molecular Modelling and chemoinformatics (8 ECTS) (O. Taboureau)** **BQ2AE160** Chemoinformatics I (J. Diharce & V.K. Tran Nguyen) (3 ECTS) **BQ2AE140** Chemoinformatics II : ADME/chemometric (O. Taboureau) (2 ECTS) **BQ2AY180** Option in drug design / Chemoinformatics (Schrödinger software, R project + EM invited professor) (3 ECTS)

SEMESTRE 2 - University Degli studi di Milano (30 ECTS)

UE1	Programming in C Or Synthetic methods in biotechnology or organics CHIM06 courses or Chemistry module (6 ECTS)	**C. Lorenzo**
UE2	Structural Biology and enzymology (6 ECTS)	**M. Vanoni**
UE3	Medicinal chemistry (6 ECTS)	**L. Belvisi**
UE4	Simulation, Modelling and Biomolecules (6 ECTS)	**S. Pieraccini**
UE5	Chemometrics (6 ECTS)	**L. Belvisi**

SEMESTRE 3 - Université Paris Cité (30 ECTS)

Block UE0 - Refresher course (L Regad)

EC000 Unix and R Basics (Upgrade) (L. Regad)
EC001 Toxicology -Methodology upgrade (A-C Camproux)

Block UE1 - Data analysis in drug design (8 ECTS) (A-C. Camproux)

EC101 Python programming 2 or Python project (S. Murail) (3 ECTS)
EC102 Data analysis in Drug Design II (A-C Camproux & L. Regad) (3 ECTS)
EC103 Application in Drug Design & QSAR (Taboureau & Regad) (1 ECTS)
EC104 Seminars and R&D (A-C Camproux) (1 ECTS)

Block UE2 - Molecular analysis and dynamics & drug design (7 ECTS) (D. Flatters)

EC201 Structural exploration of proteins (L. Regad) (3 ECTS)
EC202 Dynamic Target Analysis I (D. Flatters) (2 ECTS) or Dynamic analysis of targets II (G. Moroy) (2 ECTS)
EC203 Structural and dynamic modeling (G. Moroy & D. Flatters) (2 ECTS)

Block UE3 - Virtual screening: structure & ligand-based (5 ECTS) (G. Moroy)
EC301 Structure-based (G. Moroy) (3 ECTS)
EC302 Ligand-based (O. Taboureau) (1 ECTS)
EC303 Hits to lead (O. Taboureau) (1 ECTS)

Block UE4 - Space analysis of macromolecules (4 ECTS) (A. Badel)
EC401 Quantum chemistry (2 ECTS)
EC402 Understanding macromolecules or Data analysis I (D. Flatters) **(2 ECTS)**

Block UE5 - Preparation for research in Drug Design (6 ECTS) (L. Regad)
EC501 3-projects in Drug Design (L. Regad & O. Taboureau) (2 ECTS)
EC502 Tutored research project design (A-C Camproux) (2 ECTS)
EC503 Application of virtual screening (G. Moroy) (2 ECTS)

SEMESTRE 4 - Université Paris Cité (30 ECTS)

UE6	**STAGE (30 ECTS)** **EC 601** Tutored research project (A-C Camproux & S. Murail) (3 ECTS) **EC 602** Research internship (A-C Camproux) (27 ECTS)	**A-C. Camproux**