MASTER BIOINFORMATICS (2021-2022)
ISDD-Macromolecules research course
ISDD-Macromolecule Modeling (Initial training)

SEMESTER 1 - University of Paris (30 ECTS)

Refresher course (G. Moroy)

BQAAY000 Unix and R Basics (Upgrade) (G. Moroy & L. R egad)

Fundamentals of Biochemistry and Biostatistics (7 ECTS) (C. Etchebest)

BQAAY210 Enzymology (J. Dairou) (2ECTS)
BQAAY240 Structure of Biomolecules (N. Caulet) (2 ECTS)

BQAAY020 Biostatistics and R programming (L. Regad) (3 ECTS). **Or according to level**
BQAAY030 Tutored project in biostatistics and R (A-C Camproux & A.Badel) (3 ECTS)

Programming and mathematical tools (9 ECTS) (J.C Gelly & A. Badel) (3 EC according to level)

BQ2AY040 Mathematics I (A-C Camproux) (3 ECTS) **Or**
BQAAY060 Optimization and learning in biology (D. Flatters, F. Guyon) (3 ECTS)

BQAAY070 Python programming 1 **or**
BQAAY080 Python 2 programming (P. Fuchs & P. Poulain) (3 ECTS)

BQAAY090 Algorithmics 1 (C. Delporte, H. Fauconnier) (3 ECTS) Or
UE BQ2AC060 List of elective UE in the M1 IPFB-BIB course (to be chosen in the M1 IPFB-BIB course) (3ECTS)

Practice and deepening (8 ECTS) (O. Taboureau) ***recommended***

BQ2AY120 Systems biology & ligands, database (O. Taboureau & K. Audouze) (3 ECTS)

TX1CY090 Basics of Toxicology (A. Baeza) (3 ECTS)

BQ2AE140 ADME/chemometry (in English, O. Taboureau) (2 ECTS) *
+ **UE BQ2AU150** English (2 ECTS)

Thematic orientation I in chemistry and chemoinformatics (6 ECTS) (O. Taboureau & D. Flatters)
(2 EC to choose from)

BQ2AE160 Chemoinformatics (K. Audouze) (3 ECTS)
BQ2AE170 Chemistry: chirality - non-covalent bonds (F. Maurel, O. Taboureau) (3 ECTS)
BQ2AY180 Option for Drug Design (O. Taboureau) (3 ECTS)

SEMESTER 2 - University of Paris (30 ECTS)

Advanced fundamentals (6 ECTS) (A-C. Camproux)

BQABY010 : Massive data analysis (A-C. Camproux, A. Badel) (3 ECTS)
BQABY020: Biophysics of interactions (V. Gruber & W. Majeran) (3 ECTS)

Thematic orientation II (18 ECTS) (G. Moroy & O. Taboureau)

BQ2BY030 Protein-Protein Docking (course in English) (A-C. Camproux, O. Taboureau) (3 ECTS)
BQ2BY040 Introduction to Drug Design In Silico (G. Moroy) (3 ECTS)
BQABY050 Dynamics of macromolecules (D. Flatters, P. Fuchs) (3 ECTS)
BQ2BY060 Structural bioinformatics in Toxicology (D. Flatters, G. Moroy, O. Taboureau) (3 ECTS)
BM0BY250 Reactivity and organic synthesis (F. Chau) (3 ECTS)

Options to choose from *(* recommended)*
BQ2BY080 *In silico* practices in 3D protein complexes* (K. Moncoq, O. Taboureau) (3 ECTS)
BQ2BY090 Advanced simulation methods* (S. Murail) (3 ECTS)
BQ2BY100 Research in drug design (O. Taboureau) (3 ECTS)
UE BQ2BC110 among UE course M1BIB-IPFB (Web programming, ...) (3 ECTS)

Professionalization internship I (6 ECTS) (G. Moroy, V. Gruber, O. Taboureau)

BQ2BT130 : Internship 4 (G. Moroy, V. Gruber, O. Taboureau) (6 ECTS)

(Semester 2 of the ISDD Bioactive Molecules course)
2nd SEMESTER ERASMUS University of Milan (30 ECTS)
Or 2nd SEMESTER of study at the UNIVERSITY OF SECHENOV (MOSCOW)
in the framework of the French-Russian double degree

M2 Research course ISDD-Macromolecules

SEMESTER 3 - University of Paris (30 ECTS)

Block UE0- Refresher course (A-C. Camproux)

BQAAY010 *Unix and R Basics (Upgrade) (L. Regad)*
BQ2CY021 *Toxicology -Methodology upgrade (A-C Camproux)*

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

BQAAY070 (Python1 programming (Fuchs & P. Poulain) (3 ECTS)
Or **BQAAY080** Python programming 2 or **BQAAY030** Python project (S. Murail) (3 ECTS)
BQ2CY050 Data analysis in Drug Design (A-C Camproux & L. Regad) (3 ECTS)
BQ2CY060 Application in Drug Design & QSAR (O. Taboureau & L. Regad) (1 ECTS)
BQ2CY070 Seminars and R&D (A-C Camproux) (1 ECTS)

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

BQ2CY090 Structural exploration of proteins (L. Regad) (3 ECTS)
BQ2CY100 Dynamic analysis of targets I (D. Flatters) (2 ECTS)
Or according to level
BQ2CY110 Dynamic analysis of targets II (G. Moroy) (2 ECTS)
BQ2CY080 Structural and dynamic modeling (G. Moroy & D. Flatters) (2 ECTS)

Block UE3- High-throughput screening: structure & ligand-based (5 ECTS) (G. Moroy)

BQ2CY120 Structure-based (G. Moroy) (3 ECTS)
BQ2CY130 Ligand-based (O. Taboureau) (1 ECTS)
BQ2CY140 Hits to lead (O. Taboureau) (1 ECTS)

Block UE4- Molecular Space Analysis (4 ECTS) (O. Taboureau)

BQ2CY150 Toxicology and biotransformation (A. Baeza, F. Rodrigues-Lima) (3 ECTS)
BQ2CY160 Medicinal chemistry, pharmaceutical molecules (C. Mayer & F. Barbault) (1 ECTS)

Block UE5- Preparation to research in Drug Design (6 ECTS) (L. Regad)

BQ2CY170 3-projects in Drug Design (L. Regad & O. Taboureau) (2 ECTS)
BQ2CY180 Tutored research project design (A-C Camproux) (2 ECTS)
BQ2CY190 Application of high throughput screening (G. Moroy) (2 ECTS)

SEMESTER 4 - University of Paris (30 ECTS)

INTERNSHIP (30 ECTS) (A-C. Camproux)

UE6- **BQ2DY010** Preparation of a tutored research project (A-C Camproux & S. Murail) (3 ECTS)
UE7- **BQ2DT020** International research internship (A-C Camproux) (27 ECTS)

OR SEMESTER 4 RESEARCH INTERNSHIP (30 ECTS) at SECHENOV UNIVERSITY (MOSCOW)
as part of the French-Russian double degree