

**MASTER BIOINFORMATICS (2022-2023)**  
**ISDD-Macromolecules research course**  
**ISDD-Macromolecule Modeling (Initial training)**

**SEMESTER 1 - University Paris Cité (30 ECTS)**

**Refresher course (G. Moroy)**

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

**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 Paris Cité (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)  
2<sup>nd</sup> SEMESTER ERASMUS University of Milan (30 ECTS)  
Or 2<sup>nd</sup> SEMESTER of study at the UNIVERSITY OF SECHENOV (MOSCOW)  
in the framework of the French-Russian double degree (currently suspended)

## M2 Research course ISDD-Macromolecules

SEMESTER 3 - University Paris Cité (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 Paris Cité (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 (currently suspended)