# Fiche de renseignement UE

PAM2MIMC  UE Modélisation des interactions molécule-cible thérapeutique 1

**Description*** :

Les thématiques de l'UE sont les suivantes :

**Chemoinformatic:**

**CHEMICAL MOLECULE**

Representation and research of structures and substructures.
Similarity search (2D / 3D), clustering and diversity analysis.
Search of chemical molecules in patent databases or chemical reactions.

**MOLECULAR INTERACTIONS AND ENERGY EVALUATIONS**

Molecular interactions, molecular docking, virtual screening, molecular mechanics, molecular dynamics, QSAR.

**Molecular modelling & drug-design:**

Notions of structural biology of macromolecules. Homology modeling.

Introduction to modelling based on deep learning approach.

Structure and Ligand based drug design. Introduction to Fragment based drug-design.

**Session on modelling stations**

A case study using kinase inhibitors will allow to discover several molecular modelling tools.

Mots-clés :

Chemoinformatics & Molecular modelling.

Drug-design. Ligand- & Structure-based drug desin. Fragment based drug-design.

**Objectifs*** :

Based on theoretical knowledge of molecular interactions, elements of biochemistry and structural biology, the aim is to give students practical experience on modelling tools. The limitations and possibilities of several software programs will thus be understood.

**Volumes horaires*** :

CM : 12 H
TD :  6 H

**Pré-requis nécessaires*** :

Une licence en chimie ou biologie

**Responsables*** :

Alain Chavanieu

**Equipe pédagogique** :

Alain Chavanieu, Maxime Louet

# Fiche de renseignement UE

PAM2MIMT  UE Modélisation des interactions molécule-cible thérapeutique 2

**Description*** :

Using several therapeutic targets described in others UE ( Targeted therapies, Structure-based drug design, Drug design: case studies) applications and developments in structure-, ligand- and fragment-based drug design will be investigated.

Several practical modelling tools such as molecular dynamics, molecular docking and virtual screening will be studied through case studies.

Virtual reality for visualization and drug design in a dedicated room will allow an immersion in structural models.

*Case studies available:*

Serine protease and metallo-protease inhibitors

Phosphodiesterase inhibitors

Kinase inhibitors

Inhibitors of protein-protein interactions

Proteolysis targeting chimera (Protac) strategy against several targets

G-protein Coupled Receptors (GPCR)

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Mots-clés :

Molecular modelling.

Molecular dynamics and conformational analysis

Molecular Docking

Visualisation and drug design in Virtual Reality

Drug design

**Objectifs*** :

Direct application of the theoretical and practical knowledge acquired by the student in molecular modelling to specific examples that are widely used in therapeutic chemistry.

**Volumes horaires*** :

CM : 12 H
TD :  6 H

**Pré-requis nécessaires*** :

UE Modélisation des interactions molécule-cible thérapeutique 1

**Responsables*** :

Alain Chavanieu

**Equipe pédagogique** :

Maxime Louet & et Alain Chavanieu