UNIVERSIDAD AUTÓNOMA DE MADRID

# 33207 - DRUG DESIGN: FROM CLASSICAL TO IN SILICO

## Syllabus Information

**Code - Course title:** 33207 - DRUG DESIGN: FROM CLASSICAL TO IN SILICO

**Degree:** 721 - Máster en Investigación Farmacológica (2018)

**Faculty:** 106 - Facultad de Medicina

**Academic year:** 2019/20

## 1.Course details

### 1.1.Content area

Classical drug design based on homology of molecules with known activity and computer-aided drug design based on the three-dimensional structure of the selected pharmacological targets. Computational methods of interaction calculations and structure selection.

### 1.2.Course nature

Optional

### 1.3.Course level

Máster (MECES 3)

### 1.4.Year of study

1

### 1.5.Semester

Second semester

### 1.6.ECTS Credit allotment

5.0

### 1.7.Language of instruction

English

### 1.8.Prerequisites

General concepts of chemistry.

### 1.10.Minimum attendance requirement

It will be mandatory to attend at least 80% of the sessions.

### 1.11.Faculty data

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**Contact hours:** Previous e-mail appointment is required

### 1.12.Competences and learning outcomes

#### 1.12.1.Competences

**BASIC AND GENERAL**
GE1 - Acquire the knowledge, skills and abilities necessary to carry out an innovative quality research in Pharmacology

CB6 - Possess and understand knowledge that provides a basis or opportunity to be original in the development and / or application of ideas, often in a research context

CB7 - Know how to apply the acquired knowledge and their ability to solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their area of interest

CB9 - That the students know how to communicate their conclusions and their knowledge to specialized and non-specialized publics in a clear and unambiguous way

CB10 - Posses the learning skills that will allow the students to continue studying in a way that will be largely self-directed or autonomous.

**TRANSVERSAL**
T2 - Ability to carry out effective scientific and technical communication, both in a specialized environment and in more general environments, including the educational.

T1 - Ability to carry out a self-learning plan, perform an autonomous consultation of the bibliography and databases at the scientific, technical or regulatory level.

**SPECIFIC**
ES-3 - Know the basic aspects about the design and obtaining new drugs, both at a chemical and biotechnological level, as well as the scientific, ethical and regulatory aspects that condition it.

ES-4 - Know the most common therapeutic targets in cardiovascular disease or diseases of the nervous system and assess their physiological significance and their therapeutic projection.

### 1.12.2.Learning outcomes

Knowledge Acquisition related to the classic design of small molecules with pharmacological activity and advance in the study of new computational methodologies for computer-aided drug design, including the design of multidrug drugs. On the other hand, this knowledge will be applied to the study of the molecular interaction of known drugs on their respective therapeutic targets

### 1.13.Course contents

General aspects of the drug design process focusing on the most important approaches currently used. The course will allow the students to be able to follow medicinal chemistry research with a complementary point of view to the pharmacokinetics and pharmacodynamics subjects on the Master. The contents are designed with a theoretical and practical part. The theoretical part will be divided in the following sections.

**1. General Overview of drug design (1 h)**
- 1.1. Drug targets.
- 1.2. Protein structure and target definition.
- 1.3. Pharmacokinetics and pharmacodynamics.
- 1.4. Drug discovery, design and development.

**2. Classic drug design (4 h)**
- 2.1. Drug targets
- 2.2. Proteins: Structure and functions
- 2.3. Intermolecular bonding forces
- 2.4. Drug targets: Enzymes
- 2.5. Drug targets: Receptors
- 2.6. Drug targets: Signal transduction
- 2.7. Drug targets: Nucleic acids

**3. Drug discovery (5 h)**
- 3.1. Finding a lead compound.
- 3.2. Active compounds-based drug design.

3.3. Hybridization
3.4. Bioisosteric modification of active compounds
3.5. Quantitative Structure-activity relationships
3.6. Target interactions-based optimization
3.7. Hit-to-lead and lead to drug optimization
3.8. ADME optimization

**4. “in silico” drug design (5 h)**

4.1. Computer assisted drug design: Basics
4.2. Molecular and quantum mechanics
4.3. Protein preparation and 3D pharmacophore preparation
4.5. Molecular docking and binding energy determination
4.6. Virtual screening and data analysis.
4.7. Molecular dynamics

**Practical program (15 h)**

1. Protein data bank (PDB): Cristalographic structures of proteins, data format, 3D protein structure selection and preparation.
2. Pymol: Basic concepts, protein visualization, representation, binding site selection, protein surfaces.
3. AutoDock: Protein preparation, binding sites, ligand preparation, docking parameters, docking preparation, data analysis.
4. AutoDock: Virtual Screening.
5. AMBER: Molecular dynamics.

### 1.14.Course bibliography

- **Graham L. Patrick: An introduction to Medicinal Chemisty**: Oxford University press, 4th Edition, 2008.
- **Computational drug design**: Gore, Mohini, Jagtap, Springer, 2018.

## 2.Teaching-and-learning methodologies and student workload

### 2.1.Contact hours

| | | Nº of hours | % |
|---|---|---|---|
| Contact hours | Lectures | 15 | 33 |
| | Tutorials scheduled throughout the semester | 5 | |
| | Seminars | 5 | |
| | Practical sessions | 15 | |
| | Final examination | 1 | |
| Independent study | study | 78 | 67 |

| | | Nº of hours | % |
|---|---|---|---|
| time | Exam Preparation | 6 | |
| **Total charge of working hours: 25 hours x 5 ECTS** | | **125** | |

**2.2.List of training activities**

**LECTURES:** delivered by a professor on the topics included in the program.

**SEMINARS/TUTORIAL:** exhibition by students of problems and case studies prepared by them and included in the program. It will be followed by group discussions supervised by the tutor.

## 3.Evaluation procedures and weight of components in the final grade

### 3.1.Regular assessment

1. Continuous evaluation based on attendance and information obtained through personal tutorials, active participation in classes and seminars and skills and interest shown in class
2. Final written exam
3. Evaluation of the preparation and presentation of specific topics and discussion after their presentation by students in seminars

#### 3.1.1.List of evaluation activities

1. Continuous evaluation based on attendance and information obtained through personal tutorials, active participation in classes and seminars and skills and interest shown in class: 10%
2. Final written exam: 70%
3. Evaluation of the preparation and presentation of specific topics and discussion after their presentation by students in seminars: 20%

### 3.2.Resit

The same as for the regular assessment.

#### 3.2.1.List of evaluation activities

The same as for the regular assessment.

## 4.Proposed workplan

Schedule will be published in moodle https://moodle.uam.es/