

Curso Académico: 2022/23

## 68453 - Moléculas bioactivas: identificación, diseño y desarrollo

### Información del Plan Docente

**Año académico:** 2022/23

**Asignatura:** 68453 - Moléculas bioactivas: identificación, diseño y desarrollo

**Centro académico:** 100 - Facultad de Ciencias

**Titulación:** 626 - Máster Universitario en Biofísica y Biotecnología Cuantitativa/Biophysics and Quantitative Biotechnology

**Créditos:** 6.0

**Curso:** 01

**Periodo de impartición:** Primer semestre

**Clase de asignatura:** Obligatoria

**Materia:**

## 1. Información Básica

### 1.1. Objetivos de la asignatura

- 1 - Possess and understand knowledge that provides a basis or opportunity to be original in the development and / or application of ideas, often in a context of research
- 2 - Students should be able to apply acquired knowledge and problem-solving skills in environments new or little known within broader (or multidisciplinary) contexts related to their area of study
- 3 - Students are able to integrate knowledge and confront the complexity of making judgments from information that, incomplete or limited, includes reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments
- 4 - That the students know how to communicate their conclusions and the last knowledge and reasons that support them to specialized public and non-specialized services in a clear and unambiguous manner
- 5 - Students have the learning skills that allow them to continue studying in a way that will be largely self-directed or autonomous.

These approaches and objectives are aligned with the following Sustainable Development Goals (SDGs) of the United Nations Agenda 2030 (<https://www.un.org/sustainabledevelopment/es/>), so that the acquisition of the learning outcomes of the subject provides training and competence to contribute to some extent to their achievement: GOAL 3: GOOD HEALTH AND WELL-BEING, GOAL 4: QUALITY EDUCATION and GOAL 8: DECENT WORK AND ECONOMIC GROWTH.

### 1.2. Contexto y sentido de la asignatura en la titulación

This course will allow the students learn about:

- . Thermodynamics of equilibria and biomolecular interactions
- . Development of identification bioassays
- . Experimental and virtual screening of chemical libraries
- . Analysis of natural products
- . Toxicity, bioavailability and effectiveness tests
- . Structure / activity relationships
- . Tools for the design and engineering of proteins
- . Stabilization, optimization and design of proteins

### 1.3. Recomendaciones para cursar la asignatura

As a compulsory subject, BM is based on the knowledge acquired previously in the University Degrees that allow the students the access to this Master. Also, minimum English level is required (B2 or equivalent).

## 2. Competencias y resultados de aprendizaje

## 2.1. Competencias

- 1- Formulate the basic equations and matter balances characteristic of simple ligand protein binding equilibria.
- 2 - Design assays for the identification of substances with predetermined biological activities
- 3 - Adapt identification assays to high throughput formats to screen large collections of candidate compounds
- 4 - Apply knowledge of molecular docking (docking) to the identification of binding compounds (Pharmacological or inhibitory chaperones)
- 5 - Design procedures for the analysis of natural products aimed at the identification of the active ingredient
- 6 - Designing cell and animal assays for toxicity, bioavailability and effectiveness of bioactive compounds
- 7 - Apply statistical techniques to carry out studies that relate molecular structure with biological activity and allow the generation of predictive models
- 8 - Identify appropriate protein engineering techniques to modify or combine preexisting protein functions
- 9 - Design strategies for target protein stabilization

## 2.2. Resultados de aprendizaje

- 1 - Order, analyze critically, interpret and synthesize information
- 2 - Obtain information from different types of sources and evaluate their reliability
- 3 - Learn efficiently through autonomous study and acquire a significant degree of independence
- 4 - Apply acquired knowledge and solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to the area of study
- 5 - Formulate, analyze, evaluate and compare new or alternative solutions to different problems
- 6 - Be able to work in multidisciplinary and international teams
- 7 - Develop capacity for criticism and self-criticism
- 8 - Make decisions taking into account social, ethical and legal responsibilities
- 9 - Be able to develop a project, participating in the stages of bibliographic search, experiment planning, obtaining results, interpreting, and disseminating them

## 2.3. Importancia de los resultados de aprendizaje

- 1 - Manage in an adequate way the resources and the available time for the resolution of a problem or the development of a draft
- 2 - Communicate own conclusions and the latest knowledge and reasons that support them - to specialized audiences
- 3 - Transmit information in an oral, written or graphic form using appropriate presentation tools and with the limitations imposed by time or space
- 4 - Communicate fluently in English (understanding scientific texts, writing reports, lectures, colloquiums, exhibitions, etc.)
- 5 - Use Information and Communication (ICT) techniques as a tool for expression and communication
- 6 - Possess and understand knowledge that provides a basis or opportunity to be original in the development and/or application of ideas, often in a context of Research
- 7 - Develop technological applications of biochemical processes and transfer solutions to the industry in the food, chemical, cosmetic, pharmaceutical or health sector

## 3. Evaluación

### 3.1. Tipo de pruebas y su valor sobre la nota final y criterios de evaluación para cada prueba

Homework (35/100): Preparing a report about a topic related to the course. The report will be prepared individually or in groups of two students. It will evaluate according to the structure in sections (introduction, methodology, results, discussion, conclusions and references), considering how the student describes in a clear way the problem statement, describe properly the methodology, and the results in a logic and sequential way, give original ideas in the description, provide conclusions justified by the job and reports the appropriate the references in literature.

Written Test (50/100): It will comprise of questions that requires short or long answers. Short ones will allow performing a comprehensive sampling of the student knowledge and long ones will allow students to exhibit their expression capabilities in presentation and sustain argumentations, and critical judgments. This written test will be based on the learning activity program.

Seminars (15/100): Report preparation and public presentation and defense about a topic related to the course. This report will be individual or in two group students. The presentation sessions will have seminar format. 10-15 minutes for presentation and defense. The work will be evaluated according to its structure (coherent) and appropriate literature reference contained; clarity and tidiness during the presentation; maturity during debate.

## 4. Metodología, actividades de aprendizaje, programa y recursos

### 4.1. Presentación metodológica general

- The methodology followed in this course is oriented towards achievement of the learning objectives. It favors the understanding of the different aspects that involve the identification, design and development of bioactive molecules with application in biomedicine. A wide range of teaching and learning tasks are implemented, such as theory sessions, laboratory sessions and workshops in the computer classroom, individual assignments and seminars, workshop and discussion.
- Students are expected to participate actively in the class throughout the semester.
- Classroom materials will be available via Moodle. These include a repository of the lecture notes used in class, the course syllabus, as well as other course-specific learning materials.
- Further information regarding the course will be provided on the first day of class.

### 4.2. Actividades de aprendizaje

The course includes 6 ECTS organized according to:

- Interactive lecture sessions: (0.8 ECTS: 20 hours).
- Practical workshops in the computer lab room (0.6 ECTS): 15 hours.
- Practical individual assessments with computer (0.6 ECTS): 15 hours.
- Assignments: Presentation and work exposition or seminar (0.4 ECTS): 10 hours.
- Autonomous work (3.6 ECTS): 90 hours.

Theory sessions: 2-hour sessions take place. Lecture notes and a series of problems (and its solutions) will be available for the students. At the end of each topic, some of the problems will be solved in class by the professor and the rest will be done individually. The professor will also assign some unsolved problems to be submitted later.

Practical sessions: 3-hour sessions take place. Students are provided in advance with task guidelines for each session.

### 4.3. Programa

The course will address the following topics:

#### **Theory sessions (20 hours of theoretical lessons):**

##### **SECTION 1: Biomolecular Engineering for medicine and biotechnology**

- 1.1- Gen cloning/expression systems and protein purification process
- 1.2- Site directed and random protein mutagenesis
- 1.3- Protein modeling applications for rational design of protein mutations
- 1.4- Protein improvement: Thermostability Protein Solubility and Protein Affinity
- 1.5- Development of new enzymes
- 1.6- New commercial biological products as bioactive compounds

##### **SECTION 2: Strategies for new drug candidates? identification**

- 2.1- Drug discovery and optimization
- 2.2- Protein folding and protein/ligand binding equilibria
- 2.3- Molecular, cellular and in vivo assays during the identification of bioactive compounds
- 2.4- Experimental screening of chemical libraries
- 2.5- Computational screening of chemical libraries
- 2.6- QSAR models: structure/function relationships. Synthetic chemistry and medicinal chemistry. Development and validation of QSAR models.

##### **SECTION 3: From ?in vitro? bioactive molecules identification to ?in vivo? testing**

- 3.1- Bioavailability testing (ADME): Pharmacodynamics and pharmacokinetics
- 3.2- Drug toxicity tests in cells and animals
- 3.3- Drug targeting
- 3.4- Developing new drugs: Examples of small molecules identification

#### **Practical sessions (30 hours of practical sessions):**

Students will be guided through practical exercises to deeper understand and apply the content previously showed in the theory sessions.

#### **Seminar sessions (10 hours of students presentations):**

Students will explain a research project related to the subject topic.

#### **4.4. Planificación de las actividades de aprendizaje y calendario de fechas clave**

For further details concerning the timetable, classroom and further information regarding this course please refer to the "Facultad de Ciencias" website (<https://bioquimica.unizar.es/>).

Exams call, exams dates and academic calendar in general can be check in the webpage:

<http://ciencias.unizar.es/web/horarios.do>

Theory sessions: Monday 10:00-12:00; Tuesday 9:00-12:00; Thursday 9:00-12:00.

Practical cases, homework, oral presentations and written test will be announced.

#### **4.5. Bibliografía y recursos recomendados**

<http://psfunizar10.unizar.es/br13/egAsignaturas.php?codigo=68453>