Universidad de Navarra

Chemical Biology for Drug Discovery (MIDI)

Guía docente 2025-26

INTRODUCTION

Course: Chemical Biology for Drug Discovery

This course provides an overall view regarding the drug discovery process. The student is exposed to the multidisciplinary character of the process of the discovery of new compounds with potential therapeutic use, from the identification and design of pharmacological tools for validating new potential therapeutic targets to the optimization of said tools for their conversion into drugs.

In addition, by means of real practical cases, the critical role played by the integration of the different areas involved in the drug discovery process will be evidenced and evaluated; in other words, team work. This multidisciplinary view shows the impact that each one of the courses within the Master Program has on the identification and on the design as well as on the optimization of new molecules: biological chemistry and medicinal chemistry.

The work carried out with the aforementioned practical cases permits evaluation of the scientific maturity and critical skills as well as a multifactorial and innovating view of the student and his/her work on a team. Finally, the student's skills regarding the presentation and discussion of the case results will also be evaluated.

Degree:

Master´s Degree in Drug Research, Development and Innovation (Drug R&D&I)

Module I: Drug research

Course Area: Drug discovery

Type of course: Required

ECTS: 3

Language: English/Spanish

Responsible lecturer: Dr. Julen Oyarzabal

Lecturers: Dr. Julen Oyarzabal

Department, School: Organic and Pharmaceutical Chemistry, Pharmacy and Nutrition

Schedule: CALENDAR

LEARNING OUTCOMES (Competencies)

CB6. Poseer y comprender conocimientos que aporten una base u oportunidad de ser originales en el desarrollo y/o aplicación de ideas, a menudo en un contexto de investigación.

CG4. Identificar y saber crear estrategias y acciones dirigidas a la consecución de los objetivos planteados y concretar los recursos necesarios para llevarlas a cabo, en el ámbito de la empresa farmacéutica.

CG6. Poseer capacidad crítica para tomar las decisiones necesarias y adaptarse a las nuevas situaciones que puedan surgir en el ámbito de la empresa farmacéutica y afines.

CE1. Diseñar nuevos fármacos y terapias innovadoras para la industria farmacéutica aplicando técnicas especializadas de quimioinformática y bioinformática.

PROGRAM

Theoretical Aspects,

The objective of this class is to facilitate a general and practical view of the discovery process of new molecules. In the theoretical sessions, examples of real cases will be provided to teach the general concepts. The topics to be covered in class are as follows:

1.- Introduction.

1.1. Definition of our objective: What is a drug?

1.2. Detailed description of the drug discovery process

2.- Biological Chemistry: Identification and/or design of chemical probes for validating new potential targets of therapeutic interest.

2.1. Computational approaches to virtual screening, selection of compounds to be tested

2.2. Test strategies: From biochemical and biophysical approximations to image analysis (phenotypes)

2.3. Requirements of the optimum profile for a conclusive pharmacological tool.

3.- Medicinal Chemistry: Iterative process in drug discovery.

3.1. Identification and/or design of compounds that interact with our objective target: rational and computational approach

3.2. Selection of compounds on which a drug discovery project is based: Evaluation of their synthetic accessibility as well as their novelty (intellectual property)

3.3. Work flow design: from the primary assay and profiled ADMET *in-vitro* until the *in-vivo* assay.

3.4. Data handling. Tools for analysis and decision taking: impact on the iterative process, optimization of molecules so that can be converted into drugs.

Hands-on Training,

These practical training sessions are focused on a medicinal chemistry project currently underway, with compounds in clinical phases, and whose target has already been validated - PI3K (retrospective case study).

We will use real data from patents and articles (the student will be provided with this information). A multifactorial analysis of the information will be carried out in such a way

that will provide a comprehensive view to design new compounds with an optimum PK/PD profile:

1. Visualization and analysis of data

2. Rational design, based on prior analysis

3. Prioritization of molecules based on basic theoretical models; eg structure-based molecular design

4. Chemical viability of the proposal

5. Analysis of intellectual property (IP)

Based on guidelines described in the theoretical sessions and the retrospective case study, students will apply their knowledge to a real case scenario. Thus, students will elaborate a project proposal describing a comprehensive and feasible approach to achieve a new drug to treat an unmet medial need - different therapeutic areas will be covered.

The Chemical Computing Group. Inc. gives their permission to use their MOE software for this project. It is a standard tool within the pharmaceutical industry which facilitates data analysis (rationalize data) and also permits purely computational studies. In addition, an application (SciFinder) will be used in order to access the CAS (Chemical Abstracts Service) database of the American Chemical Society where the majority of the existing chemical compounds are listed - evaluation of the novelty of the proposals (IP).

Acknowledgements:

School of Pharmacy, University of Navarra, thanks Chemical Computing Group (www.chemcomp.com) for providing free access to their software "MOE" to perform these practical sessions.

EDUCATIONAL ACTIVITIES

3 ECTS x 25h= 75 horas

Theoretical classes: 14 hours (0.56 ECTS)

Practical Classes: 18 hours (0.72 ECTS)

Evaluation: 2 hours (0.08 ECTS)

Individual work: 41 hours (1.64 ECTS)

ASSESSMENT

ORDINARY EXAMINATION

The final grade will be based on the following: 10% of the grade obtained from project proposal, 10% of the grade obtained from the personal hands-on work, 40% of the grade obtained from project defense and 40% of the grade obtained on the written exam.

1. Defending the project proposal, 15 minutes (10%)

The objective is to make a project proposal: Therapeutic Area, Indication & Target

The student must perform a bibliographic analysis to select, based on proposed guidelines and current research articles, a project. This proposal is the starting point for the "hands-on" project.

2.- Personal hands-on work (10%)

The student must be involved in the daily work required to design, develop and implement an optimal project; individual performance, as part of the team work, will be assessed during hands-on training sessions.

3. Defending the "hands-on" project, 15 minutes (40%)

The objective is to present the current state of the research project that the student has directed. The student must explain the state of the project and the steps to follow in order to meet the objective: what, how and where.

The student must show the impact of the retrospective analysis carried out (data available up to now) as well as the use of different prospective approaches that led to the specific proposals carried out and the strategy used to carry them out.

4. Written exam, 45 minutes (40%)

This exam is made up of 2 written development questions. The questions cover that which was taught in the theoretical as well as practical program.

RE-SIT EXAMINATION

Students who do not pass in the ordinary exam (minimum score of 5 out of 10), must re-sit an exam with the same characteristics previously mentioned in the ordinary exam.

OFFICE HOURS

The students make an appointment for personalized counseling by sending an e-mail to:

- Dr. Julen Oyarzabal (teacher responsible for this subject), julenoyarzabal@external.unav.es
- Dr. Pablo Garnica (teacher), pgarnica@unav.es

BIBLIOGRAPHY AND RESOURCES

MOE sofware will be available durign the hands-on sessions at the PCs in CTI, at this point we would like to thank Chemical Computing Group

(https://www.chemcomp.com) for providing free acces to their software "MOE" to perform these sessions.

Some books of interest:

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1.- The practice of medicinal chemistry [Electronic resource] / edited by Camille Georges Wermuth. Amsterdam; Boston: Elsevier/Academic Press, 2008. (4rd edition). Find it in the Library (ebook)

2.- Burger's medicinal chemistry and drug discovery. Vol. I, Principles and practice / edited by Manfred E. Wolff. New York [etc.] : Wiley & Sons, cop. 1995. 5th edition. Find it in the Library

3.- Molecular Modelling: Principles and Applications (2nd Edition), by Andrew R. Leach, Prentice Hall. Find it in the Library

4.- An Introduction to Chemoinformatics (Revised Edition), by Leach A.R., Gillet V.J. Springer, 2007. Find it in the Library