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Academic Year of Degree: 2025/26

## 24044 - Introduction to Drug Research and Development

### Teaching Guide Information

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**Academic Course:** 2025/26

**Academic Center:** 337 - Engineering School

**Study:** 3378 - Bachelor's degree in Biomedical Engineering

**Subject:** 24044 - Introduction to Drug Research and Development

**Credits:** 4.0

**Course:** 4

**Teaching languages:**

Theory: Group 1: English

Practice: Group 101: English

Group 102: English

Seminar: Group 101: English

**Teachers:** Ismael Zamora Rico, Andres Ozaita Mintegui, Manuel Pastor Maeso, Miguel Angel Mayer Pujadas, Pablo Villoslada Diaz, Marta Barniol Xicota, Janet Piñero Gonzalez

**Teaching Period:** First term

### Presentation

Developing a new drug for a disease or clinical condition is a long and complex process. In this course, we aim to provide the student with an overview of the steps in the development of a drug from the earliest phases of drug discovery and the use of advanced computational methods commonly used to support pharmaceutical I+D, to the early stages of the drug discovery and validation and the development of the final product that can be then protected/patented and taken to the market.

Estimated time spent on the subject: 100 h

### Associated skills | General learning outcomes

#### General competences

A general understanding of the different stages of drug discovery from initial target identification and validation, through assay development, high throughput screening, hit identification, lead optimization, the selection of a candidate molecule for clinical development, phases of clinical trials and final drug approval.

### Specific competences

Understanding the field of application of most common experimental and computational methods within the drug-discovery pipeline

Understanding the language of other professionals (medicinal chemist, pharmacologist) working in the drug discovery and development field

### Learning outcomes | Specific learning outcomes

Student successfully completing this course:

- Have a general understanding of the drug discovery and development process
- Know and understand different experimental and computational methods in the drug discovery and development process (advantages and limitations). Critically rationalize and interpret data linked to those methods.
- Have the skills to communicate efficiently with other professionals involved in the field of drug discovery and development

### Contents

The course content is divided into four Units, starting with a general introduction to the subject (Unit 1) and providing essential background for drug discovery and research (Unit 2) that is required to understand the course and following blocks covering the most common methodologies (Unit 3-4).

#### Block 1: Introduction to drug discovery and development

**1.1. Drugs/Medicines:** definition, social and economical importance, main actors. Medicines versus APIs (active pharmaceutical ingredients), drug administration, treatment

**1.2. Overview of the drug R&D "pipeline":** target discovery and validation, hit identification, lead optimization, preclinical drug development, clinical drug development, post-marketing monitoring

#### Block 2: Foundations of drug discovery

**2.1. Notions of medicinal chemistry:** organic molecules, drug-likeness, chirality, charge, identifiers

**2.2. General mechanisms of drug action:** drug-receptor interaction, targets for drug action, molecular and cellular aspects of drug action, sensitization and desensitization, quantitative aspects of drug-receptor interaction

**2.3. Notions of experimental pharmacology:** in vitro and in vivo pharmacology, agonist/antagonist, dose-response relationship, potency and efficacy concepts, drug distribution and bioavailability, concepts of IC<sub>50</sub>, K<sub>i</sub>, K<sub>d</sub>, LD<sub>50</sub>, therapeutic index

**2.4. Notions of knowledge management in pharmaceutical research:** sources

of relevant information for pharmaceutical research. Open source vs proprietary sources. Walkthrough by several highly relevant sources (ChEMBL, DrugBank, Open PHACTS, etc.). Open PHACTS API.

**2.5. Notions of pharmacokinetics:** overview of the physiological processes involved in the Absorption, Distribution, Metabolism and Elimination of drugs. Importance and implication of ADME for the development of new drugs. Experimental and computational tools used for assessing the druggability of candidates from the point of view of their ADME properties.

**2.6. Notions of drug safety assessment:** strategies for drug safety assessment, non-clinical, preclinical, clinical

### Block 3: Discovery and preclinical drug development

**3.1. Identification of potential cancer drug targets using cancer genomics data:** Recent advances in DNA sequencing technologies provide unprecedented capacity to comprehensively identify mutations, genes, and pathways involved in the tumorigenic process, raising the hope of extending targeted therapies from a few successful examples to a broader personalized medicine strategy. In the lecture I will explain how to explore cancer genomics data to identify potential new cancer drug targets.

**3.2. Drug target validation:** druggable target, pharmacological approaches, genetic approaches (antisense oligonucleotides, RNAi, transgenic animals), caveats: splice variants, multimeric receptors, one gene>one protein>one drug target.

**3.3. High throughput screening in drug discovery:** compound libraries (natural compounds, corporate compounds), in silico screening, rational drug design, combinatorial chemistry, physical substrates in HTS, biochemical based assays and cell-based assays.

**3.4. Structure-based approaches in drug discovery I:** generation of 3D models, geometry optimization, ligand docking, de-novo drug design, fragment-based approaches

**3.5. Structure-based approaches in drug discovery II:** docking, chemoisosterism, target profiling

**3.6. In silico prediction of drug properties:** in silico prediction of drug properties, concept of molecular similarity and bioisosterism, concept of QSAR, applications of in silico prediction in drug development: structural alerts, read across, QSAR and QSPR

**3.7. Integrative knowledge management:** exploitation in drug discovery and development, including multi-level and multi-scale modelling and simulation.

### Block 4: Clinical Development

**4.1. Testing drugs in humans:** an introduction to clinical trials: This lecture will be devoted to explain the main reasons that justify the research in humans during the process of drug development. It will introduce the concept of clinical trial, their different types and its sequential use along the development of new and old drugs.

**4. 2. The basis of clinical trial methodology:** This lecture will introduce the attendees to the main characteristics of the methodological approach of clinical trials. Special focus will be on the process of randomization, blinding procedures, definition of outcomes, experimental biases and data analysis.

**4.3. Ethical compromises in clinical trials:** This lecture will include a historical analysis of how human research was carried out in the past, which justified the definition of bioethical principles applied to such situations. A short review of the current legal status of clinical trials will also be considered.

**4.4. Taking drugs to the market:** Overview of the steps required for registering a NCI and obtaining the approval of the main international drug regulators (FDA, EMA). Marketing considerations.

**4.5. Pharmacovigilance:** Follow-up of marketed drugs by the health authorities. Declaration of human adverse effects. Potential implications and reasons for drug market withdrawal.

## **Sustainable Development Goals**

- 3 - Good Health and Well-being
- 4 - Quality Education
- 5 - Gender Equality
- 8 - Decent Work and Economic Growth

## **Evaluation and grading system**

### **Assessment system**

The students are evaluated using two instruments:

- (A) Evaluation of their participation in seminars and hands-on/practice sessions through specific deliverables from each session, and
- (B) A multiple-choice questionnaire (35-40 questions) about the concepts in the theory and seminar sessions. A minimum score of 5 out of 10 is necessary to pass this exam and make the average for the final marks.

Students not reaching the overall pass grade (5 out of 10 score) will be allowed to retake a written test in July, that will be evaluated using the same criteria applied to the first test.

#### **Grading system**

The relative weight of the two above instruments in the final mark is 40% for A (the seminars and hands-on/practice) and 60% for B (the multiple-choice questionnaire).

Final marks will range from 0 to 10.

A minimum grade of 5.0 is required to pass the course.