PHARMACOLOGY: DRUG DESIGN

Tishk International University
Faculty of Applied Science
Medical Analysis Department

Lecture – 6
Second Semester
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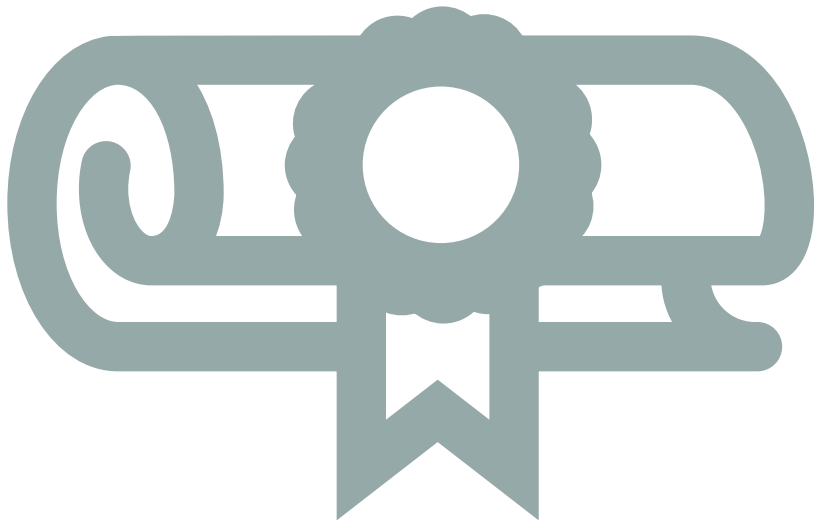
Course Description

This course introduces the fundamental principles of pharmacology, focusing on:

- Drug classification systems
- Mechanisms of drug action
- Pharmacokinetics (ADME)
- Pharmacodynamics
- Drug–drug interactions
- Toxicology and drug safety

Week	Topic
1	Introduction to Pharmacology
2	Pharmacokinetics (ADME)
3	Pharmacodynamics
4	Steroid & Non-Steroid Drugs
5	Nervous System Pharmacology
6	Cardiovascular Pharmacology
7	Antimicrobial Agents
8	Endocrine & Metabolic Drugs
9	Hematology & Chemotherapy
10	General Toxicology
11	Clinical Toxicology & Drug Safety
12	Student Presentations & Review

COURSE SYLLABUS



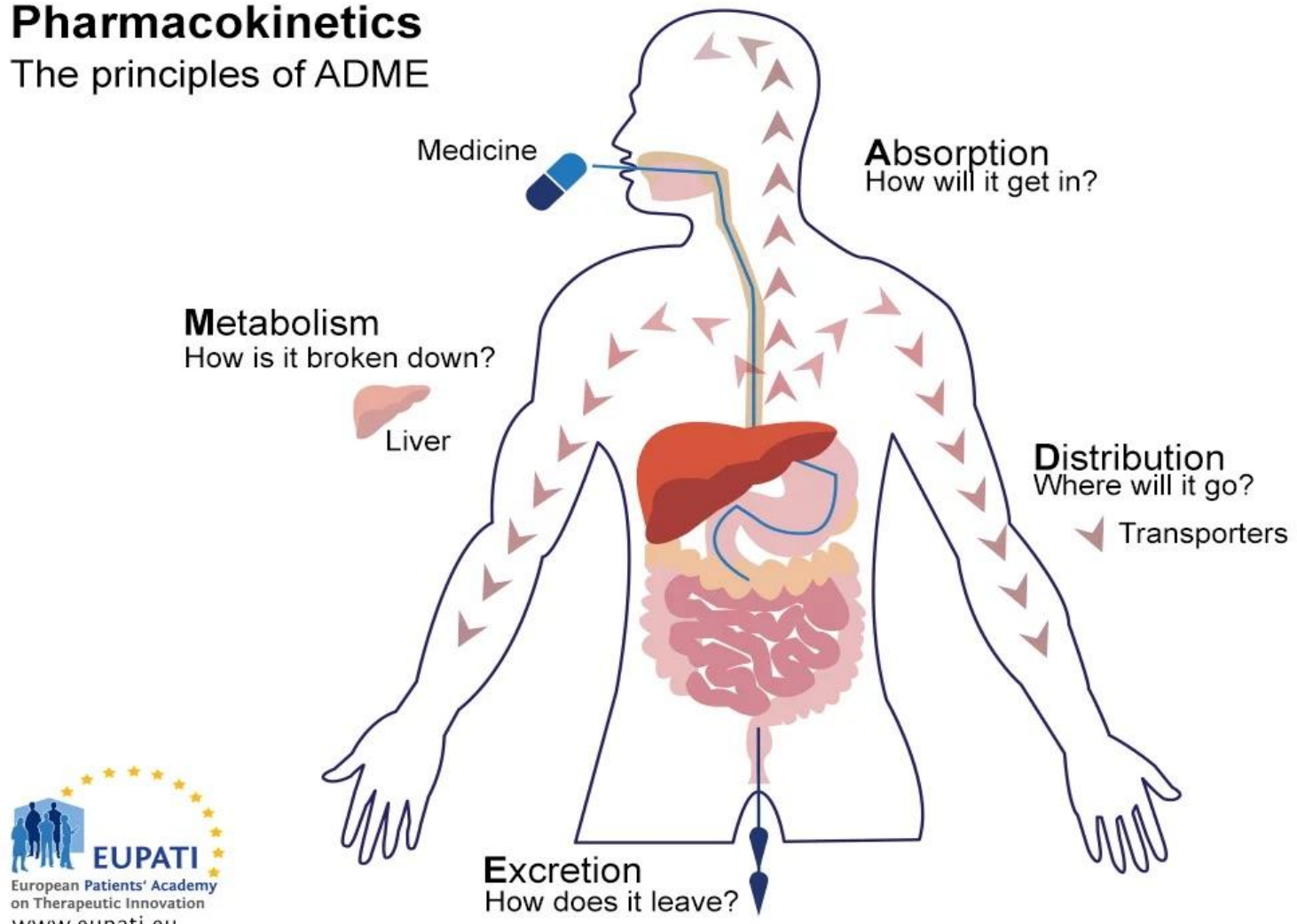
Outline

- Definition and introduction
- Classification
- Mechanism of action

Learning Objectives

- Drug design & development
- Drug testing in pre-clinical research
- Clinical Pharmacology
- Cancer Chemotherapy

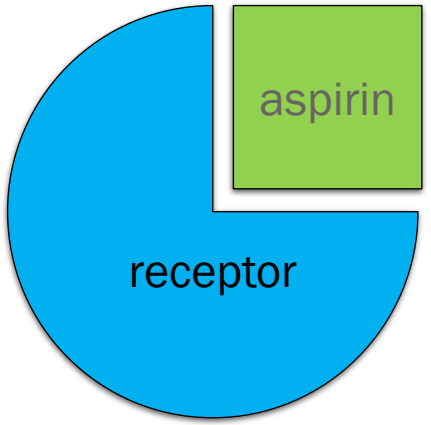
Pharmacokinetics



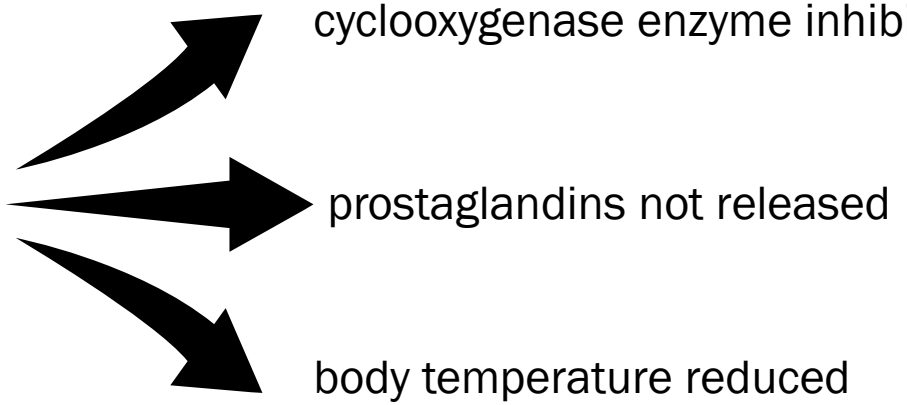
Pharmacodynamics

Pharmacodynamics studies the drug's effect on the body & the mechanisms of its action.

DRUG-RECEPTOR BINDING



POST-RECEPTOR EFFECT

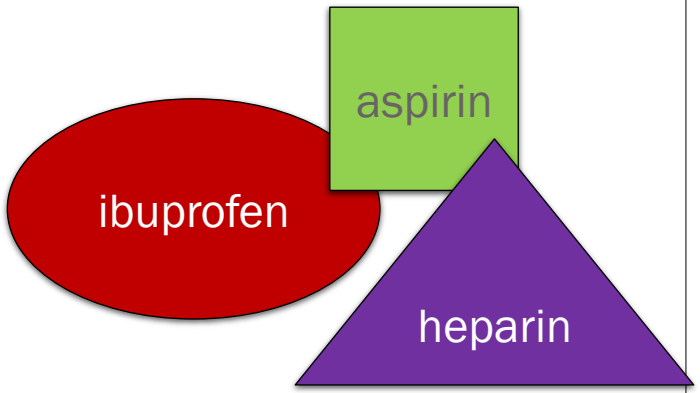


cyclooxygenase enzyme inhibited

prostaglandins not released

body temperature reduced

DRUG INTERACTION



Clinical Pharmacology

Steps in drug research

Design & development

Drug testing

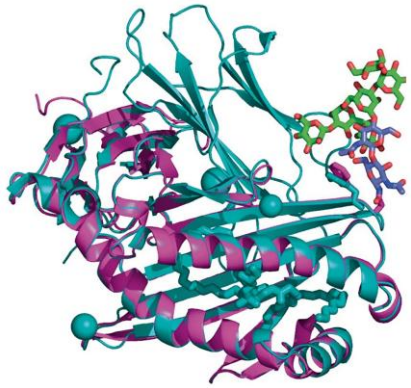
Drug certification

Drug design & development

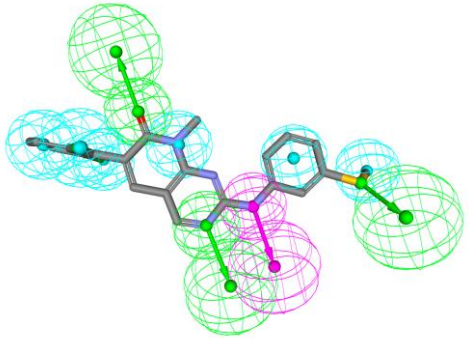
Steps in Drug Design & Development

1. Choose a disease

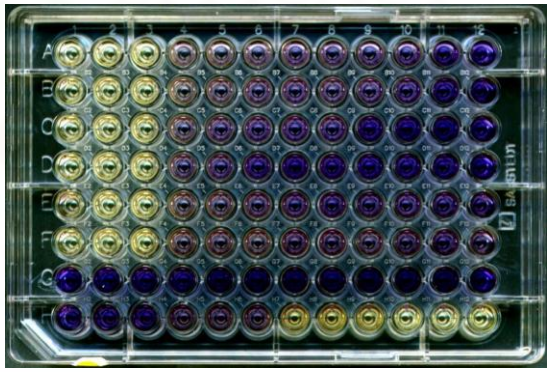
2. Identify drug target



3. Find a lead compound



4. Choose an assay



Drug design & development

Choose a Disease

- Pharmaceutical companies are commercial enterprises.
- Pharmaceutical companies, therefore, tend to avoid products with a small market, i.e. a disease which only affects a small subset of the population.

Drug design & development

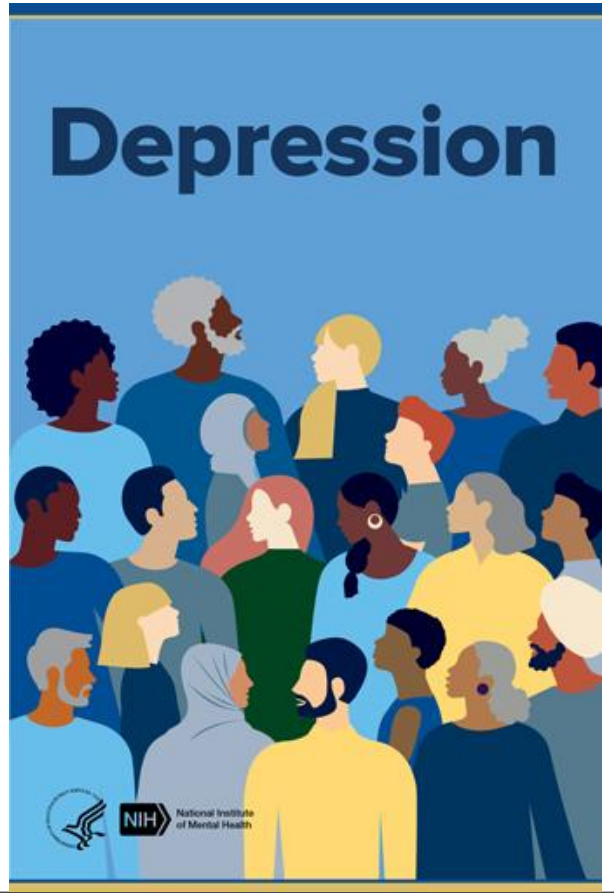
Choose a Disease

- Pharmaceutical companies avoid products consumed by individuals of lower economic status, i.e. a disease which only affects third-world countries.

Drug design & development

Choose a Disease

- Most research is carried out on diseases that affect the “first world” countries, e.g. cancer, cardiovascular diseases, depression, diabetes, flu, migraine, obesity, etc.



Drug design & development

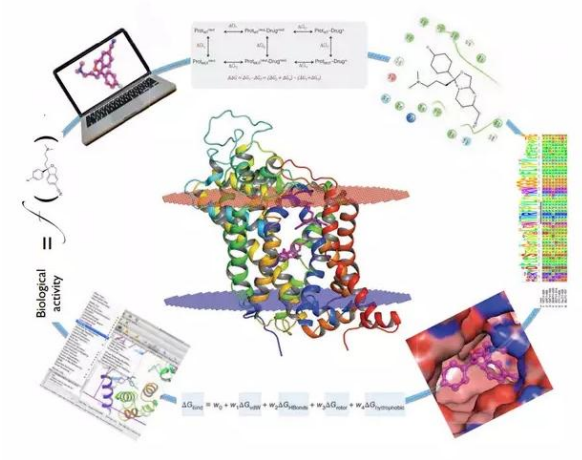
Identify Drug Target

A drug target is a specific macromolecule, or biological system, with which the drug will interact. A target can be a protein, RNA, DNA, modified sugars, etc.

- Some targets are in the **human body** (non-infectious & infectious diseases).
- Some targets are in the **pathogen** (infectious diseases).
- In pharmacological history, many targets were found **incidentally.**

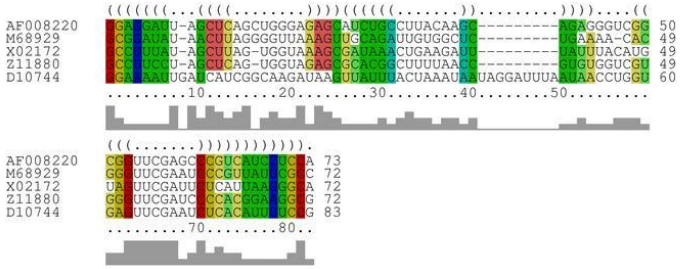
Drug design & development

- Computer modelling



- Genomic libraries

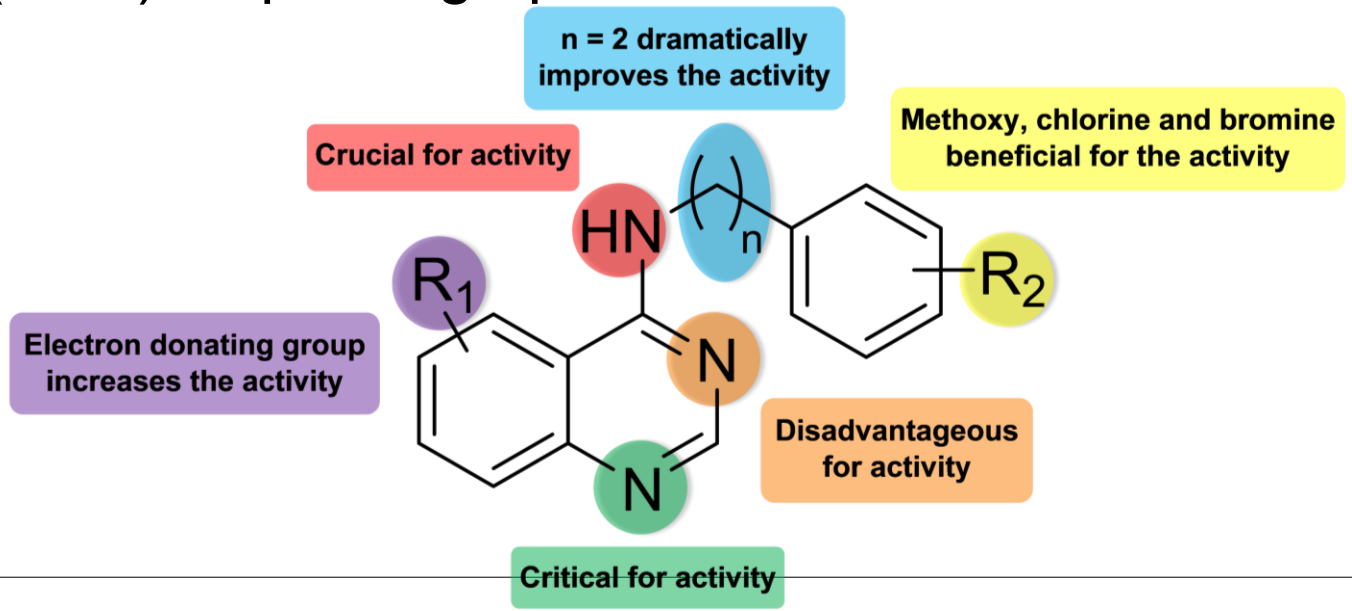
- Alignment techniques



Drug design & development

A lead compound is a chemical with some activity against the chosen target but is not yet good enough to be the drug.

- If not known, computer modelling and AI can help determine the structure of the lead compound.
- Structure-Activity Relationship (SAR) helps drug optimization.

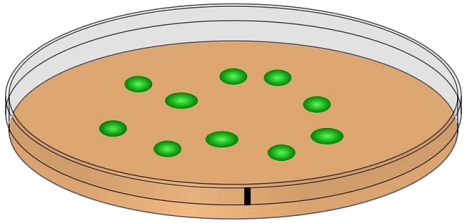


Drug design & development

Choose an Assay

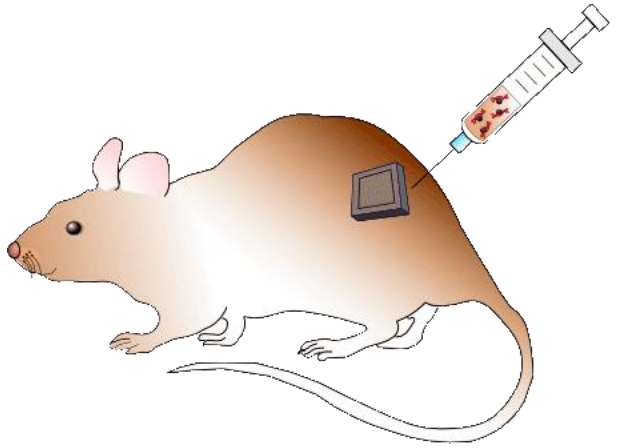
In vitro

- in an artificial environment, e.g. in a test tube or culture plate



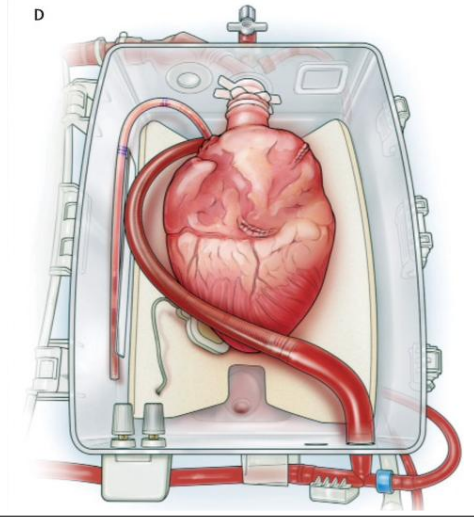
In vivo

- in the living body, e.g. in living animals



Ex vivo

- on a tissue taken from a living organism



Cancer chemotherapy

- **Cancer chemotherapy** is the use of cytotoxic drugs to kill or inhibit the growth of malignant cells.
- Unlike surgery or radiotherapy, chemotherapy is systemic, meaning it can target primary tumors and metastatic disease.

Key Principles:

- Targets rapidly dividing cells
- Affects both cancer and normal proliferating cells (bone marrow, GI tract, hair follicles)
- Often used in combination regimens to improve efficacy and prevent resistance

Cancer chemotherapy

Goals of Chemotherapy:

- Curative (e.g., leukemia, lymphoma)
- Control disease progression
- Palliative (symptom relief)

Classification of Chemotherapeutic Agents

Chemotherapy drugs are classified based on mechanism of action and chemical structure:

Class	Mechanism of Action	Cell Cycle Specificity	Key Examples	Major Toxicities
Alkylating Agents	DNA cross-linking → inhibits replication & transcription	Non-specific	Cyclophosphamide, Cisplatin	Myelosuppression, nephrotoxicity (cisplatin)
Antimetabolites	Mimic nucleotides → inhibit DNA/RNA synthesis	S-phase specific	Methotrexate, 5-Fluorouracil	Myelosuppression, mucositis
Antitumor Antibiotics	DNA intercalation, free radical formation	Mostly non-specific	Doxorubicin, Bleomycin	Cardiotoxicity (doxorubicin), pulmonary toxicity (bleomycin)
Microtubule Inhibitors	Disrupt mitotic spindle → block mitosis	M-phase specific	Vincristine, Paclitaxel	Neurotoxicity, myelosuppression
Topoisomerase Inhibitors	Inhibit DNA unwinding → DNA breaks	S/G2 phase	Etoposide	Myelosuppression
Hormonal Therapy	Block hormone receptors or synthesis	Phase-independent	Tamoxifen	Thromboembolism, endocrine effects
Targeted Therapy & Immunotherapy	Target specific molecular pathways or immune checkpoints	Variable	Trastuzumab	Cardiotoxicity, immune-related effects

Cell Cycle Specificity

Drug Type	Phase
Antimetabolites	S-phase
Microtubule inhibitors	M-phase
Alkylating agents	Non-specific

Combination Chemotherapy

Why combine drugs?

- Different mechanisms
- Reduce resistance
- Increase tumor cell kill

Principles:

- Use non-overlapping toxicity
- Target different cell cycle phases

References

- Katzung Basic & Clinical Pharmacology
- Goodman & Gilman's The Pharmacological Basis of Therapeutics
- Jawetz, Melnick, & Adelberg's Medical Microbiology
- World Health Organization