

MEDICINAL CHEMISTRY I

Code number: ΝΠ18-35

Cycle: Undergraduate

Semester: 5

Course type

	Background/General knowledge
X	Scientific area (pharmacy)

Credit Units (ECTS): 7

Lectures (hours/week): 3

Tutorial (hours/week):

Laboratory work (hours/week): 2

Course coordinator:

Vassilis Demopoulos, Professor

Tutor (s):

Vassilis Demopoulos, Professor

Room 408/A & 409/B, 4th floor Biology/Pharmacy building.

Collaboration with students: Every day.

Communication: e-mail (vdem@pharm.auth.gr)

Antonis Gavalas, ΕΔΙΠ

Room 407/A, 4th floor Biology/Pharmacy building.

Collaboration with students: Every day.

Communication: e-mail (agavalas @pharm.auth.gr)

Assisting personnel:

Aims of the course:

- Relationship between structure-physicochemical properties and action of drug molecules
- Chemical-molecular mechanism of action of drug molecules
- Chemical stability of drug molecules
- Biotransformations of xenobiotics
- Representative synthetic strategy-Chemical quantitative identification of drug molecules

Skills:

Practical application of heterocyclic ring formation in anhydrous and thermodynamically controlled conditions. Authentication and purity check by thin layer chromatography. Chemical quantification of xenobiotics using: a) alkaline hydrolytic methodology, b) various redox methodologies, and c) reactions in anhydrous conditions.

Teaching methods: Lectures

Contents of the course:

Tutors:

1) Vassilis Demopoulos

Introduction to the chemistry of vitamins. Pharmacochemical study of vitamins. Composition / isolation / analysis, physicochemical properties, absorption / action and uses of water-soluble vitamins (e.g. thiamine, folic acid, nicotinic acid, nicotinamide, ascorbic acid) as well as fat-soluble vitamins (e.g. tocopherols, vitamin K). Presentation of related drugs (i.e. sulfanilamides, isoniazid, and anticoagulant coumarins). Synthetic strategy, origin - isolation, structural characterization, analysis, absorption and molecular mechanism of action, structure-activity relationships,

selectivity, pharmacochemical aspects of activity and fate in the organism of the following groups of drugs: histamine agonists (H1 and H2), histamine antagonists (H1 and H2), antibacterial, antifungal and antiviral chemotherapeutics.

2) Antonis Gavalas

Synthetic strategy, origin - isolation, structural characterization, analysis, absorption and molecular mechanism of action, structure-activity relationships, selectivity, pharmacochemical aspects of activity and fate in the organism of the following groups of drugs: acidic and non-acidic NSAIDs (non-steroidal anti-inflammatory drugs) as well as anti-gout drugs.

Proposed literature:

1. Βασίλης Ι. Δημόπουλος "ΦΑΡΜΑΚΕΥΤΙΚΗ ΧΗΜΕΙΑ- Ομάδες Χημειοθεραπευτικών και Φαρμακοδυναμικών Φαρμάκων", Θεσσαλονίκη 2002, ISBN 960-317-063-1 (Εύδοξος)
2. "Vitamins", 2005 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, ISBN 10.1002/14356007.a27 443
3. Joseph J. Cannon "Pharmacology for Chemists", Oxford University Press, 2007, ISBN-10: 0841239274.
4. R.B. Silverman "The Organic Chemistry of Drug Design and Drug Action", 2nd ed., 2004, Academic Press.
5. E. J. Corey, B. Czako, L. Kurti "Molecules and Medicine", Wiley, 2007, ISBN-10: 0470227494

Educational activities: Lectures, discussion with the students in every lecture.

Evaluation process and methods: Examination is performed at the end of the semester. To compute the final grade, the grade which is given by each tutor is added
The duration of the examination is 3 hours.
The examination at the end of the semester is performed at dates, time and place arranged by the department.

Use of TIC / Electronic distribution of the lectures

Lectures, notes, statements etc are presented in the website: <http://users.auth.gr/vdem/>.

Teaching: Teaching of this course is accomplished through lectures laboratory work.

- A) **Lectures.** Lectures (39 in total, three hours per week) are given in the lecture room D12 (main building of the School of Natural Sciences)

Lecture	Title	Tutor
1-3	Introduction / definition of vitamins. Folic acid and its coenzyme. Physicochemical properties, chemical stability, absorption, deficiency, complement, toxicity, and synthetic strategy in the preparation of folic acid. Presentation of sulfanilamides as related drugs.	V. Demopoulos
4-5	Relationships of structure / physicochemical properties and activity of sulfanilamides. Synthetic manufacturing strategy, chemical quantification, and their biotransformations.	V. Demopoulos

B)

6-8	Niacin and its coenzymes. Physicochemical properties, chemical stability, absorption, deficiency, complement, toxicity, and synthetic strategy in the preparation of niacin. Presentation of isoniazid as a related drug.	V. Demopoulos
9-12	Ascorbic acid and α -Tocopherol as free radical scavengers and coenzymes. Physicochemical properties, chemical stability, absorption, deficiency, supplement, toxicity and synthetic manufacturing strategy of these vitamins. Chemical quantification of ascorbic acid.	V. Demopoulos
13-15	Vitamin K and Thiamine. Their coenzymes. Physicochemical properties, chemical stability, absorption, deficiency, supplement, toxicity, and synthetic strategy for the preparation of vitamin K and thiamine.	V. Demopoulos
16-17	Presentation of coumarins as related to vitamin K anticoagulants.	V. Demopoulos
18-22	NASAIDs (acidic and non-acidic). Structure / physicochemical properties and activity relationships, synthetic manufacturing strategy, chemical quantification, and their biotransformations.	A. Gavalas
23-24	Anti-gout drugs, chemical biology of pharmacodynamic / pharmacokinetic behavior, methods of retrosynthetic preparation & physicochemical identification.	A. Gavalas
25-27	Histamine agonists (H1 and H2), histamine antagonists (H1 and H2). Physicochemical parameters and selectivity in the action of ligands on histamine receptors.	V. Demopoulos
28	Chemotherapeutic drugs, selective toxicity, antibacterial antibiotics, penicillins, structural & physicochemical parameters in the molecular mechanism of their activity	V. Demopoulos
29-30	Synthetic strategy towards benzylpenicillin, nafcillin, carbenicillin & ampicillin.	V. Demopoulos
31-32	Cephalosporins, stereochemical characteristics & action, semi-synthetic preparation of 7-ACA.	V. Demopoulos
33-34	Other antibacterial antibiotics with molecular focus on monobactams, chloramphenicol, cycloserine, tetracyclines, aminoglycosides & macrolides.	V. Demopoulos
35-36	Non-antibiotic antibacterials with molecular focusing on, metronidazole, nitrofurantoin, & quinolones.	V. Demopoulos
37-39	Antifungal phenacyl imidazolew. Antiviral chemotherapeutics with focusing on acyclovir.	V. Demopoulos

Laboratory work.

Students are required to perform laboratory exercises (two hours / week).

CAUTION! Students, in order to practice in the laboratory, they must submit an application to the Laboratory of Pharmaceutical Chemistry. Before the beginning of the semester, a relevant announcement is posted on the bulletin board of the Laboratory of Pharmaceutical Chemistry.

Laboratory	Title	Tutors
1-5	Assignment of laboratory benches, general information, and determination of sulfanilamide	V. Demopoulos & A. Gavalas
6-9	Synthesis of himechromone	V. Demopoulos & A. Gavalas
10-13	Determination of acetylsalicylic acid	V. Demopoulos & A. Gavalas
14-17	Determination of ascorbic acid	V. Demopoulos & A. Gavalas
18-21	Determination of diphenhydramine hydrochloride by anhydrous titration.	V. Demopoulos & A. Gavalas
22-26	Identification and purity assessment of compounds by thin layer chromatography.	V. Demopoulos & A. Gavalas