

**Federal State Autonomous Educational Institution of Higher Education "Moscow
Institute of Physics and Technology
(National Research University)"**

APPROVED
**Head of the Phystech School of
Biological and Medical Physics**
D.V. Kuzmin

Work program of the course (training module)

course: Organic Chemistry and Fundamentals of Stereochemistry/Органическая химия и основы стереохимии

major: Biotechnology

specialization: Medical Biotechnology/Медицинская биотехнология
Phystech School of Biological and Medical Physics
Center for educational programs in bioinformatics

term: 1

qualification: Master

Semester, form of interim assessment: 1 (fall) - Exam

Academic hours: 90 AH in total, including:

lectures: 60 AH.

seminars: 30 AH.

laboratory practical: 0 AH.

Independent work: 60 AH.

Exam preparation: 30 AH.

In total: 180 AH, credits in total: 4

Author of the program: M.I. Medvedeva, candidate of chemical sciences

The program was discussed at the Center for educational programs in bioinformatics 24.02.2020

Annotation

The main targets of the subject studying are related to getting the knowledge of the main concepts of theoretical organic chemistry, current methods of synthesis of organic compounds, methods for qualitative control, structure, and reaction reactive capability of organic compounds as well as methods of conformational analysis of organic compounds.

1. Study objective

Purpose of the course

Exploration of theoretical fundamentals of organic chemistry as well as establishment of knowledge related to contemporary concepts of spatial structure of organic compounds.

Tasks of the course

The main targets of the subject studying are related to getting the knowledge of the main concepts of theoretical organic chemistry, current methods of synthesis of organic compounds, methods for qualitative control, structure, and reaction reactive capability of organic compounds as well as methods of conformational analysis of organic compounds. Studying of this subject creates a theory base for concurrent successful exploration of the pull of general subjects such as chemistry of high molecular mass compound, biochemistry, structure of compounds, chemistry of colloids etc. as well as specific disciplines. The received knowledges will become a certain base for continuous qualitative and deep exploration of the following disciplines as “Medicinal Chemistry: fundamental concepts and modern approaches”, “Bioorganic chemistry” as well as for preparation, carrying-out, achievement, and review of qualified projects of the students. Also, for successful solution of R&D, scientific and research, design-and-engineering, engineering and manufacturing tasks in future professional career.

2. List of the planned results of the course (training module), correlated with the planned results of the mastering the educational program

Mastering the discipline is aimed at the formation of the following competencies:

Code and the name of the competence	Competency indicators
Gen.Pro.C-3 Select and/or develop approaches to professional problem-solving with consideration to the limitations and specifics of different solution methods	Gen.Pro.C-3.1 Analyze problems, plan research strategy to achieve solution(s), propose, and combine solution approaches
	Gen.Pro.C-3.2 Employ research methods to solve new problems and apply knowledge from various fields of science (technology)
	Gen.Pro.C-3.3 Gain knowledge of analytical and computational methods of problem-solving, understand the limitations for applying the obtained solutions in practice
	Gen.Pro.C-3.4 Professionally operate and upgrade modern bioinstrumentation
	Gen.Pro.C-3.5 Has the skills to design new bioinformatics solutions for the scientific, technical, biotechnological task at hand
Gen.Pro.C-4 Successfully perform a task, analyze the results, and present conclusions, apply knowledge and skills in the field of physical and mathematical sciences and ICTs	Gen.Pro.C-4.1 Apply ICT knowledge and skills to search for and study scientific literature, using software products
	Gen.Pro.C-4.2 Apply knowledge in the field of physical and mathematical sciences to solve problems, make conclusions, and evaluate the obtained results
	Gen.Pro.C-4.3 Justify the chosen method of scientific research
	Gen.Pro.C-4.4 Evaluate, analyze, and interpret the results of biotechnological processes
	Gen.Pro.C-4.5 Set scientific and technical objectives, using biotechnological processes and the proper equipment

3. List of the planned results of the course (training module)

As a result of studying the course the student should:

know:

Classification and nomenclature of organic compounds, the most important classes of organic compounds - structure, methods of preparation, physical and chemical properties, basic theoretical concepts in organic chemistry, mutual transformations of classes of organic compounds, as well as the subject of stereochemistry, basic principles of the theory of stereochemistry, conformational analysis of organic compounds.

be able to:

Draw up a scheme for the multi-stage synthesis of an organic compound, use reference, review and monographic literature in the field of organic chemistry. Students must also have the skills to navigate various hypotheses and the theory of conformational analysis, as well as be able to depict the spatial structure of various organic molecules.

master:

- skills of mastering a large amount of information;
- skills of independent work in the laboratory and the Internet;
- skills of competent processing of experience results and comparison with theoretical data;
- practice of research and solving theoretical and applied problems.

4. Content of the course (training module), structured by topics (sections), indicating the number of allocated academic hours and types of training sessions

4.1. The sections of the course (training module) and the complexity of the types of training sessions

№	Topic (section) of the course	Types of training sessions, including independent work			
		Lectures	Seminars	Laboratory practical	Independent work
1	Introduction to Organic Chemistry	6	3		6
2	Alkanes	6	3		6
3	Alicyclic compounds	6	3		6
4	Alkenes	6	3		6
5	Alkynes	6	3		6
6	Alcadienes	6	3		6
7	Arenes	6	3		6
8	Electrophilic substitution reactions in the aromatic series	6	3		6
9	Nucleophilic substitution reactions in the aromatic series	6	3		6
10	Halogenated hydrocarbons	6	3		6
AH in total		60	30		60
Exam preparation		30 AH.			
Total complexity		180 AH., credits in total 4			

4.2. Content of the course (training module), structured by topics (sections)

Semester: 1 (Fall)

1. Introduction to Organic Chemistry

The subject of organic chemistry and the main stages of its development. Methods for depicting molecules of organic compounds, structural and electronic formulas. Organic chemistry at the present stage. Types of carbon skeleton, acyclic, cyclic and heterocyclic compounds. Molecular models. Isomerism and its types. Homology. Main functional groups. Classification of organic compounds. Oxidation state and oxidative level.

2. Alkanes

Homologous series, isomerism and nomenclature. Natural sources of alkanes are oil and gas. Methanogenesis in nature. Fischer-Tropsch process.

Synthesis methods: hydrogenation of unsaturated hydrocarbons, synthesis through lithium dialkyl cuprates, electrolysis of carboxylic acid salts (Kolbe reaction), reduction of carbonyl compounds from haloalkanes (Wurtz reaction, protolysis of Grignard reagents). The nature of C-C and C-H bonds in alkanes. Conformations of ethane, propane, butane and higher alkanes. Energy diagram of the conformational state of an alkane molecule.

3. Alicyclic compounds

Cycloalkanes and their derivatives. Classification of alicycles. Tension energy of cycloalkanes and its quantitative assessment based on a comparison of the heats of formation and heats of combustion of cycloalkanes and the corresponding alkanes. Types of stress in cycloalkanes and division of cycles into small, medium cycles and macrocycles. Structure of cyclopropane, cyclobutane, cyclopentane, cyclohexane. Conformational analysis of cyclohexane. Axial and equatorial bonds in the "chair" conformation of cyclohexane. Bicyclic and polycyclic compounds, fused, bridged, spiro compounds. Decalin (cis, trans), norbornane. An idea of natural polycyclic systems of terpenes and steroids. Frame compounds: adamantane, cubane, prism, tetrahedron. Catenanes and rotaxanes.

Methods for the synthesis of cyclopropane, cyclobutane and their derivatives. Features of the chemical properties of compounds with a three-membered ring. Synthesis of compounds of the cyclopentane and cyclohexane series. Synthesis of compounds with medium and large ring sizes (ester and acyloin condensations).

4. Alkenes

Homologous series, isomerism and nomenclature. Geometric isomerism (cis-, trans- and Z-, E-nomenclature). The nature of the double bond. Molecular orbitals of ethylene. Synthesis methods: elimination of hydrogen halides from alkyl halides, water from alcohols, dehalogenation of vic-dihaloalkanes, ammonium salts (Hoffmann reactions). Wittig reaction, stereoselective reduction of alkynes. McMurry's reaction. Heck reaction

5. Alkynes

Homologous series, nomenclature and isomerism. The nature of the triple bond. Triple bond in a small cycle. Methods for the synthesis of alkynes using elimination reactions and alkylation of terminal acetylenes. Production of acetylene by pyrolysis of methane.

6. Alcadienes

Types of dienes. Isolated, cumulated and conjugated dienes. Isomerism and nomenclature. Stereochemistry of 1,3-disubstituted allenes. Relative stability of isomeric dienes. Methods for the synthesis of cumulenes and 1,3-dienes: opening of dibromocyclopropanes, dehydrogenation of alkanes, Favorsky-Reppe synthesis, homo-coupling and cross-coupling reactions on metal complex catalysts. Butadiene-1,3, structural features. Molecular orbitals of 1,3-dienes. Chemical properties of 1,3-dienes. Halogenation and hydrohalogenation of 1,3-dienes. Allyl cation. 1,2- and 1,4-addition, thermodynamic and kinetic control. Epoxidation, cyclopropanation, hydroboration. Diels-Alder reaction with alkenes and alkynes, stereochemistry of the reaction and its application in organic synthesis, dienes and dienophiles. Structural and electronic requirements for participation in the Diels-Alder reaction. Specific properties of 1,4- and 1,5-dienes. Cyclization of butadiene on metal complex catalysts. Polymerization of dienes-1,3. The structure of rubbers and modern problems in the chemistry of elastomers.

7. Arenes

Aromaticity concept. Aromaticity. The structure of benzene. Kekule's formula. Molecular orbitals of benzene. annulled. Aromatic and non-aromatic annulenes. Frost Circle. Aromaticity concept. Hückel's rule. Aromatic cations and anions. Non-benzenoid aromatic systems - cyclopropenyl cation, cyclopentadienyl anion, tropylium cation, cyclooctatetraene dianion. Condensed aromatic hydrocarbons: naphthalene, phenanthrene, anthracene, azulene, etc. Heterocyclic five- and six-membered aromatic compounds (pyrrole, furan, thiophene, pyridine). Antiaromaticity using the example of cyclobutadiene, cyclopropenyl anion, and cyclopentadienyl cation. Aromaticity criteria (magnetic, structural, energetic).

8. Electrophilic substitution reactions in the aromatic series

Classification of aromatic electrophilic substitution reactions. General understanding of the reaction mechanism, kinetic isotope effect in reactions of electrophilic substitution of hydrogen in the benzene ring. The idea of π - and σ -complexes. Arenonium ions in electrophilic substitution reactions. Influence of the nature of the substituent on the orientation and rate of the electrophilic substitution reaction. Electron-donating and electron-withdrawing substituents. Consistent and inconsistent orientation of two or more substituents in the benzene and naphthalene series. Orientants of the first and second kind.

9. Nucleophilic substitution reactions in the aromatic series

Bimolecular mechanism S_NAr substitution in the series of halogenarenes, substitution of the nitro group. Activating groups and orientation. Meisenheimer complexes. The concept of fluoroquinolone antibiotics. Hydride ion substitution followed by oxidation (NASH). Vicarious nucleophilic substitution, examples of reactions with nitrobenzene, amination using hydroxylamine. Arine mechanism, structure and reactivity of dehydrobenzene (regiochemistry of addition of nucleophiles, reactions with dienes, synthesis of tryptcene), methods of synthesis from halogenbenzenes, o-aminobenzoic acid, concept of heteroaromatic and polyaromatic derivatives of dehydrobenzene. Anion-radical mechanism SRN synthetic capabilities, mechanism. Monomolecular mechanism for diazonium salts $SN1$. Catalysis by Pd and Ni complexes.

10. Halogenated hydrocarbons

Isomerism, nomenclature. Methods of production from alcohols, alkanes, alkenes; replacement of one halogen atom with another, chloromethylation of arenes.

5. Description of the material and technical facilities that are necessary for the implementation of the educational process of the course (training module)

- classrooms for lecture-type lessons;
- auditoriums equipped with computer equipment with connection to the Internet;
- computer and multimedia equipment (projector, sound system),
- individual computing facilities of students (personal computers) for doing homework.

6. List of the main and additional literature, that is necessary for the course (training module) mastering

Main literature

This literature is provided by the base department

1. Реутов, О.А. Органическая химия [Текст]: В 4 ч.: Ч.: 4: Учебное пособие для вузов / О.А. Реутов, А.Л. Курц, К.П. Бутин - М.: Бином, 2004-2009.
2. Травень, В.Ф. Органическая химия. [Текст]: в 2 т./ В.Ф. Травень - М.: Издательско-книготорговый центр Академкнига, 2008. - 2 т.
3. Смит, В.А. Основы современного органического синтеза [Текст]: уч. пособие для вузов / В.А. Смит, А.Д. Дильман - М.: Бином. Лаборатория знаний, 2009. - 750 с.
4. Джоуль, Дж. Химия гетероциклических соединений [Текст] (пер. с англ. языка) / Дж. Джоуль, К. Миллс - М.: Мир, 2004. - 728с. - ISBN 5-03-003461-7, 0-632-05453-0.
5. Илиел, Э. Основы органической стереохимии. [Текст] (пер. с англ. языка) / Илиел Э., Вайлен С., М. Дойл - М.: Бином. Лаборатория знаний, 2007. - 704с. - ISBN 978-5-94774-370-8, 0-471-37499-7.

Additional literature

7. List of web resources that are necessary for the course (training module) mastering

Immunobiology, 5th edition (NCBI bookshelf). <http://www.ncbi.nlm.nih.gov/books/NBK10757/>
Англоязычная Википедия. <http://en.wikipedia.org/>

8. List of information technologies used for implementation of the educational process, including a list of software and information reference systems (if necessary)

For some of the lessons, you will need Zoom. Google Drive to access course materials. The presence of smartphones / laptops during classes is encouraged to participate in interactive exercises.

9. Guidelines for students to master the course

The section provides instructions on organizing the student's activities in mastering the discipline: preparing for lecture and seminar classroom classes, independent work, recommendations on the optimal organization of the process of studying the educational material of the discipline, links to the methodological sections of the department's website, a list of guidelines used in the educational process on this discipline.

Assessment funds for course (training module)

major: Biotechnology
specialization: Medical Biotechnology/Медицинская биотехнология
Phystech School of Biological and Medical Physics
Center for educational programs in bioinformatics
term: 1
qualification: Master

Semester, form of interim assessment: 1 (fall) - Exam

Author: M.I. Medvedeva, candidate of chemical sciences

1. Competencies formed during the process of studying the course

Code and the name of the competence	Competency indicators
Gen.Pro.C-3 Select and/or develop approaches to professional problem-solving with consideration to the limitations and specifics of different solution methods	Gen.Pro.C-3.1 Analyze problems, plan research strategy to achieve solution(s), propose, and combine solution approaches
	Gen.Pro.C-3.2 Employ research methods to solve new problems and apply knowledge from various fields of science (technology)
	Gen.Pro.C-3.3 Gain knowledge of analytical and computational methods of problem-solving, understand the limitations for applying the obtained solutions in practice
	Gen.Pro.C-3.4 Professionally operate and upgrade modern bioinstrumentation
	Gen.Pro.C-3.5 Has the skills to design new bioinformatics solutions for the scientific, technical, biotechnological task at hand
Gen.Pro.C-4 Successfully perform a task, analyze the results, and present conclusions, apply knowledge and skills in the field of physical and mathematical sciences and ICTs	Gen.Pro.C-4.1 Apply ICT knowledge and skills to search for and study scientific literature, using software products
	Gen.Pro.C-4.2 Apply knowledge in the field of physical and mathematical sciences to solve problems, make conclusions, and evaluate the obtained results
	Gen.Pro.C-4.3 Justify the chosen method of scientific research
	Gen.Pro.C-4.4 Evaluate, analyze, and interpret the results of biotechnological processes
	Gen.Pro.C-4.5 Set scientific and technical objectives, using biotechnological processes and the proper equipment

2. Competency assessment indicators

As a result of studying the course the student should:

know:

Classification and nomenclature of organic compounds, the most important classes of organic compounds - structure, methods of preparation, physical and chemical properties, basic theoretical concepts in organic chemistry, mutual transformations of classes of organic compounds, as well as the subject of stereochemistry, basic principles of the theory of stereochemistry, conformational analysis of organic compounds.

be able to:

Draw up a scheme for the multi-stage synthesis of an organic compound, use reference, review and monographic literature in the field of organic chemistry. Students must also have the skills to navigate various hypotheses and the theory of conformational analysis, as well as be able to depict the spatial structure of various organic molecules.

master:

- skills of mastering a large amount of information;
- skills of independent work in the laboratory and the Internet;
- skills of competent processing of experience results and comparison with theoretical data;
- practice of research and solving theoretical and applied problems.

3. List of typical control tasks used to evaluate knowledge and skills

Physical and physicochemical research methods in organic chemistry

Carboxylic acids and their derivatives

Amines

Diazo compounds

Nitro compounds
Phenols and quinones
Heterocyclic compounds
Amino acids, peptides, and proteins
Carbohydrates
Metal complex catalysis

4. Evaluation criteria

1. Introduction to Organic Chemistry
2. Alkanes
3. Alicyclic compounds
4. Alkenes
5. Alkynes
6. Alkadienes
7. Arenes
8. Electrophilic substitution reactions in the aromatic series
9. Nucleophilic substitution reactions in the aromatic series
10. Halogenated hydrocarbons
11. Elimination reactions
12. Organometallic compounds
13. Hydroxy derivatives of hydrocarbons
14. Ethers
15. Aldehydes and ketones

The mark is excellent (10 points) - given to a student who has shown comprehensive, systematized, deep knowledge of the curriculum of the discipline, who is interested in this subject area, who has demonstrated the ability to confidently and creatively apply them in practice in solving specific problems, free and correct justification of the decisions made.

The mark is excellent (9 points) - given to a student who has shown comprehensive, systematized, in-depth knowledge of the curriculum of the discipline and the ability to confidently apply them in practice when solving specific problems, free and correct justification of decisions made.

The mark is excellent (8 points) - given to a student who has shown comprehensive, systematized, deep knowledge of the curriculum of the discipline and the ability to confidently apply them in practice when solving specific problems, the correct justification of the decisions made, with some drawbacks.

The mark is good (7 points) - given to a student if he firmly knows the material, expresses it competently and in essence, knows how to apply the knowledge gained in practice, but does not correctly justify the results obtained.

The mark is good (6 points) - given to the student if he knows the material well, expresses it competently and in essence, knows how to apply the knowledge gained in practice, but makes some inaccuracies in the answer or in solving problems.

A good mark (5 points) is given to a student if he basically knows the material, expresses it competently and in essence, knows how to apply the knowledge gained in practice, but makes a sufficiently large number of inaccuracies in the answer or in solving problems.

The mark is satisfactory (4 points) - given to a student who has shown a fragmentary, scattered nature of knowledge, insufficiently correct formulations of basic concepts, violation of the logical sequence in the presentation of the program material, but at the same time he has mastered the main sections of the curriculum necessary for further education, and can apply the obtained knowledge modeled on a standard situation.

The mark is satisfactory (3 points) - given to a student who has shown a fragmentary, scattered nature of knowledge, makes mistakes in the formulation of basic concepts, breaks the logical consistency in the presentation of program material, has poor command of the main sections of the curriculum necessary for further education and hardly applies the knowledge gained even in a standard situation.

The mark is unsatisfactory (2 points) - given to a student who does not know most of the main content of the curriculum of the discipline, makes gross errors in the formulation of basic principles and does not know how to use the knowledge gained in solving typical problems.

The mark is unsatisfactory (1 point) - given to a student who does not know the main content of the curriculum of the discipline, makes gross errors in the formulation of the basic concepts of the discipline, and generally does not have the skills to solve typical practical problems.

5. Methodological materials defining the procedures for the assessment of knowledge, skills, abilities and/or experience

When conducting an oral exam, the student is given 60 minutes to prepare. Questioning a student on a ticket during an oral exam should not exceed one astronomical hour.