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

APPROVED
Head of Landau Phystech-School of Physics & Research
A.V. Rogachev

Work program of the course (training module)

course:	Structure and Dynamics of Membrane Proteins by NMR/Структура и динамика мембранных белков методом ЯМР
major:	Applied Mathematics and Physics
specialization:	General and Applied Physics/Общая и прикладная физика
	Landau Phystech-School of Physics & Research
	Chair of Biophysics
term:	1
qualification:	Master

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

Academic hours: 30 AH in total, including:
lectures: 15 AH.
seminars: 15 AH.
laboratory practical: 0 AH.

Independent work: 15 AH.

In total: 45 AH, credits in total: 1

Number of course papers, tasks: 2

Author of the program: I.V. Manukhov, doctor of biological sciences

The program was discussed at the Chair of Biophysics 19.06.2023

Annotation

The discipline "Structure and dynamics of membrane proteins by NMR" is a specialized course of the professional cycle of academic disciplines of the biophysical profile of LFI training, which introduces students to the tools of modern high-resolution NMR spectroscopy. Students will learn best practices and learn about the most important advances of the method as applied to the life sciences.

1. Study objective

Purpose of the course

To acquaint students with the tools of modern high-resolution NMR spectroscopy. Students will learn best practices and learn about the most important advances of the method as applied to the life sciences.

Tasks of the course

1) the formation of basic knowledge about the fundamental structure of a modern NMR spectrometer and key achievements from the moment the method appeared to the present;

2) teaching students to interpret the one-dimensional proton and carbon NMR spectrum for molecules with a mass of 50-300 Da;

3) teaching students to establish the chemical structure of a molecule according to NMR spectroscopy and mass spectrometry;

4) teaching students to perform sequential signal assignment for isotopically labeled proteins.

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
UC-1 Use a systematic approach to critically analyze a problem,and develop an action plan	UC-1.1 Systematically analyze the problem situation, identify its components and the relations between them
	UC-1.2 Search for solutions by using available sources
Gen.Pro.C-1 Gain fundamental scientific knowledge in the field of physical and mathematical sciences	Gen.Pro.C-1.1 Apply fundamental scientific knowledge in the field of physical and mathematical sciences
	Gen.Pro.C-1.2 Consolidate and critically assess professional experience and research findings
Gen.Pro.C-2 Acquire an understanding of current scientific and technological challenges in professional settings, and scientifically formulate professional objectives	Gen.Pro.C-2.1 Assess the current state of mathematical research within professional settings
	Gen.Pro.C-2.2 Assess the relevance and practical importance of research in professional settings
	Gen.Pro.C-2.3 Understand professional terminology used in modern scientific and technical literature and present scientific results in oral and written form within professional communication
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-4.2 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
Pro.C-1 Assign, formalize, and solve tasks, develop and research mathematical models of the studied phenomena and processes, systematically analyze scientific problems and obtain new scientific results	Pro.C-1.3 Apply theoretical and/or experimental research methods to a specific scientific task and interpret the obtained results
Pro.C-2 Organize and conduct scientific research and testing independently or as a member (leader) of a small research team	Pro.C-2.1 Plan and conduct scientific research independently or as part of a research team
Pro.C-3 Use research and testing equipment (devices and installations, specialized software)	Pro.C-3.1 Understand the operating principles of the equipment and specialized software

(devices and installations, specialized software) in a selected subject field	Pro.C-3.3 Evaluate the accuracy of the experimental (numerical) results

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

As a result of studying the course the student should:

know:

1) Possibilities of modern NMR spectroscopy, advantages and limitations of the method;
2) The main types of NMR experiments, be able to use them in your work;
3) Strategy for working with low molecular weight compounds by NMR;
4) Strategy for working with water-soluble and membrane proteins by NMR.

be able to:

1) Use the basic laws of natural science disciplines in professional activities;
2) work with scientific and technical information;
3) identify and systematize the main ideas in scientific texts;
4) critically evaluate any incoming information, regardless of the source;
5) when solving research and practical problems, generate new ideas.

master:

1) Skills in choosing methods and means for solving research problems;
2) methods of theoretical and experimental research;
3) search skills (including using information systems and databases), processing, analysis and systematization of information;
4) the skills of critical analysis and evaluation of modern scientific achievements.

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 NMR Spectroscopy	2	2		2
2	NMR of low molecular weight compounds	2	2		2
3	NMR of proteins and the structure of biopolymers	2	2		2
4	NMR spectrum processing (signal processing)	3	3		3
5	Dynamic processes in NMR	3	3		3
6	Molecular mechanisms of the biological function of proteins by NMR	3	3		3
AH in total		15	15		15
Exam preparation		0 AH.			
Total complexity		45 AH., credits in total 1			

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

Semester: 1 (Fall)

1. Introduction to NMR Spectroscopy

Creation of the method in the middle of the twentieth century. Key stages in the evolution of NMR: superconducting high-field magnets, Fourier-NMR, two-dimensional and multidimensional NMR spectroscopy, isotope labeling, cryogenically cooled sensors.

2. NMR of low molecular weight compounds

Analysis of the proton NMR spectrum: chemical shift, integral, multiplicity. Limitations of proton NMR. Two-dimensional NMR on the natural abundance of isotopes: COZY, TOCSY, HSQC, HMBC spectra. Selection of spin systems, spectrum analysis algorithm. Combined use of NMR spectroscopy and high resolution mass spectrometry to establish the chemical structure of low molecular weight compounds.

3. NMR of proteins and the structure of biopolymers

Strategies for working with native and isotopically labeled proteins. Sequential assignment of signals, characteristic spin systems of 20 amino acids. Close, middle and far NOE contacts, features of alpha-helical and beta-structural proteins in NMR spectra. Calculation of protein structure according to NMR data.

4. NMR spectrum processing (signal processing)

Limitation of the classical Fourier transform when registering high-dimensional spectra. Strategies for incomplete sampling (NUS, Non-Uniform Sampling), their optimization. Methods for reconstructing the NMR signal from incomplete data.

5. Dynamic processes in NMR

Relaxation of nuclear spins. Relationship between relaxation and molecular size and intramolecular dynamics. Chemical/conformational exchange.

6. Molecular mechanisms of the biological function of proteins by NMR

NMR Heteronuclear NMR spectroscopy as a method of integrative structural biology and biophysics. Structural and dynamic properties of proteins and their biological function. Conformational rearrangements and structural and functional determinants of proteins. Intermolecular interactions of proteins in the membrane and their role in intercellular signaling. Examples of molecular mechanisms of protein function in normal conditions and in diseases of the body (neurodegenerative and oncogenic).

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

Classroom with a media projector and screen, Internet access.

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

Main literature

1. Методы в молекулярной биофизике: структура, функция, динамика [Текст] : в 2 т. : учеб. пособие для вузов / И. Сердюк, Н. Заккаи, Дж. Заккаи .— М. : КДУ, 2009 .— Т. 1. - 2009. - 568 с.
2. Методы в молекулярной биофизике: структура, функция, динамика [Текст] : в 2 т. : учеб. пособие для вузов / И. Сердюк, Н. Заккаи, Дж. Заккаи .— М. : КДУ, 2009 .— Т. 2. - 2009. - 736 с.
3. Масс-спектрометрия в органической химии [Текст] : учеб. пособие для вузов / А. Т. Лебедев .— М. : БИНОМ. Лаб. знаний, 2009 .— 493 с.
4. Введение в курс спектроскопии ЯМР [Текст] = NMR spectroscopy/Х. Гюнтер , -М., Мир, 1984

5. J. Cavanagh (2006) «Protein NMR Spectroscopy. Principles and Practice», Academic Press.
6. Mass spectrometry basics. Eds. C.G. Herbert, R.A.W. Johnstone. 2003 CRC Press.
7. New and emerging proteomic techniques. Eds. D. Nedelkov, R.W. Nelson, Methods in molecular biology, 328. 2006, Humana Press.
8. "Proteomics of human body fluids: principles, methods, and applications" Ed: Visith Thongboonkerd. 2007, Humana Press.
9. LC-MS/MS in Proteomics. Eds. P.R. Citillas and J.F. Timms, Methods in molecular biology, 2010, Humana Press.

Additional literature

1. ЯМР в одном и двух измерениях [Текст] = Principles of nuclear magnetic resonance in one and two dimensions/Б. Эрнст, Дж. Боденхаузен, А. Вокаун , -М., Мир, 1990
2. Э. Дероум. Современные методы ЯМР для химических исследований. Москва, Мир, 1992.

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

Открытые базы данных химической и медико-биологической информации (Chembl, drugbank, gencards, pubmed, GEO)

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

When preparing and conducting lectures, the Internet is used.
In addition, Libre Office is used, as well as the Ink Scape graphics package.

9. Guidelines for students to master the course

A student studying the discipline must, on the one hand, master the general conceptual apparatus, and on the other hand, must learn to apply theoretical knowledge in practice.
As a result of studying the discipline, the student must know the basic definitions and concepts, be able to apply the knowledge gained to solve various problems.
Successful completion of the course requires:
- attendance of all classes provided for by the curriculum for the discipline;
- keeping a synopsis of classes;
- student's intense independent work.

Independent work includes:
- reading recommended literature;
- study of educational material, preparation of answers to questions intended for independent study;
- solving problems offered to students in the classroom;
- preparation for the performance of tasks of the current and intermediate certification.

An indicator of mastery of the material is the ability to answer questions on the topics of the discipline without a synopsis.
It is important to achieve an understanding of the material being studied, not its mechanical memorization. If a student finds it difficult to study certain topics, questions, he/she should seek advice from a teacher.
Intermediate control of students' knowledge is possible in the form of solving problems in accordance with the topic of classes.

SUPPLEMENT

Assessment funds for course (training module)

major:	Applied Mathematics and Physics
specialization:	General and Applied Physics/Общая и прикладная физика Landau Phystech-School of Physics & Research Chair of Biophysics
term:	1
qualification:	Master

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

Author: I.V. Manukhov, doctor of biological sciences

1. Competencies formed during the process of studying the course

Code and the name of the competence	Competency indicators
UC-1 Use a systematic approach to critically analyze a problem,and develop an action plan	UC-1.1 Systematically analyze the problem situation, identify its components and the relations between them
	UC-1.2 Search for solutions by using available sources
Gen.Pro.C-1 Gain fundamental scientific knowledge in the field of physical and mathematical sciences	Gen.Pro.C-1.1 Apply fundamental scientific knowledge in the field of physical and mathematical sciences
	Gen.Pro.C-1.2 Consolidate and critically assess professional experience and research findings
Gen.Pro.C-2 Acquire an understanding of current scientific and technological challenges in professional settings, and scientifically formulate professional objectives	Gen.Pro.C-2.1 Assess the current state of mathematical research within professional settings
	Gen.Pro.C-2.2 Assess the relevance and practical importance of research in professional settings
	Gen.Pro.C-2.3 Understand professional terminology used in modern scientific and technical literature and present scientific results in oral and written form within professional communication
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-4.2 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
Pro.C-1 Assign, formalize, and solve tasks, develop and research mathematical models of the studied phenomena and processes, systematically analyze scientific problems and obtain new scientific results	Pro.C-1.3 Apply theoretical and/or experimental research methods to a specific scientific task and interpret the obtained results
Pro.C-2 Organize and conduct scientific research and testing independently or as a member (leader) of a small research team	Pro.C-2.1 Plan and conduct scientific research independently or as part of a research team
Pro.C-3 Use research and testing equipment (devices and installations, specialized software) in a selected subject field	Pro.C-3.1 Understand the operating principles of the equipment and specialized software
	Pro.C-3.3 Evaluate the accuracy of the experimental (numerical) results

2. Competency assessment indicators

As a result of studying the course the student should:

know:

1) Possibilities of modern NMR spectroscopy, advantages and limitations of the method;
2) The main types of NMR experiments, be able to use them in your work;
3) Strategy for working with low molecular weight compounds by NMR;
4) Strategy for working with water-soluble and membrane proteins by NMR.

be able to:

1) Use the basic laws of natural science disciplines in professional activities;
2) work with scientific and technical information;
3) identify and systematize the main ideas in scientific texts;
4) critically evaluate any incoming information, regardless of the source;
5) when solving research and practical problems, generate new ideas.

master:

1) Skills in choosing methods and means for solving research problems;
2) methods of theoretical and experimental research;
3) search skills (including using information systems and databases), processing, analysis and systematization of information;
4) the skills of critical analysis and evaluation of modern scientific achievements.

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

In order to control the students' mastery of the training material, an oral questioning is conducted at the beginning of the lesson on the topic of the last session.

4. Evaluation criteria

Checking questions:

1. Basic principles of NMR, solvent, chemical shift, multiplicity, integral
2. Fourier NMR, 2D NMR spectroscopy, NOESY, COSY, TOCSY, HSQC, HMBC
3. Methods for determining the structure of low molecular weight compounds, NMR/mass
4. spectrometry/chemical synthesis
5. Features of protein NMR spectroscopy, isotopic labeling, limitations of the method
6. Techniques for assigning signals in protein spectraMethods for obtaining the structure of proteins from NMR data: sources of information about the structure in spectra, methods for calculating the structure
7. NMR relaxation and mobility, study of equilibrium kinetics and thermodynamics of processes by NMR spectroscopy
8. Strategies of incomplete sampling (NUS, Non-Uniform Sampling), their optimization.
9. Relationship between relaxation and molecular size and intramolecular dynamics. Chemical/conformational exchange.
10. Methods for assigning signals in protein spectraMethods for obtaining the structure of proteins from NMR data: sources of information about the structure in the spectra, methods for calculating the structure.
11. NMR relaxation and mobility, the study of equilibrium kinetics and thermodynamics of processes by NMR spectroscopy.
12. Conformational rearrangements and structural and functional determinants of proteins. Intermolecular interactions of proteins in the membrane and their role in intercellular signaling.

Assessment “excellent (10)” is given to a student who has displayed comprehensive, systematic and deep knowledge of the educational program material, has independently performed all the tasks stipulated by the program, has deeply studied the basic and additional literature recommended by the program, has been actively working in the classroom, and understands the basic scientific concepts on studied discipline, who showed creativity and scientific approach in understanding and presenting educational program material, whose answer is characterized by using rich and adequate terms, and by the consistent and logical presentation of the material;

Assessment “excellent (9)” is given to a student who has displayed comprehensive, systematic knowledge of the educational program material, has independently performed all the tasks provided by the program, has deeply mastered the basic literature and is familiar with the additional literature recommended by the program, has been actively working in the classroom, has shown the systematic nature of knowledge on discipline sufficient for further study, as well as the ability to amplify it on one’s own, whose answer is distinguished by the accuracy of the terms used, and the presentation of the material in it is consistent and logical;

Assessment “excellent (8)” is given to a student who has displayed complete knowledge of the educational program material, does not allow significant inaccuracies in his answer, has independently performed all the tasks stipulated by the program, studied the basic literature recommended by the program, worked actively in the classroom, showed systematic character of his knowledge of the discipline, which is sufficient for further study, as well as the ability to amplify it on his own;

Assessment “good (7)” is given to a student who has displayed a sufficiently complete knowledge of the educational program material, does not allow significant inaccuracies in the answer, has independently performed all the tasks provided by the program, studied the basic literature recommended by the program, worked actively in the classroom, showed systematic character of his knowledge of the discipline, which is sufficient for further study, as well as the ability to amplify it on his own;

Assessment “good (6)” is given to a student who has displayed a sufficiently complete knowledge of the educational program material, does not allow significant inaccuracies in his answer, has independently carried out the main tasks stipulated by the program, studied the basic literature recommended by the program, showed systematic character of his knowledge of the discipline, which is sufficient for further study;

Assessment “good (5)” is given to a student who has displayed knowledge of the basic educational program material in the amount necessary for further study and future work in the profession, who while not being sufficiently active in the classroom, has nevertheless independently carried out the main tasks stipulated by the program, mastered the basic literature recommended by the program, made some errors in their implementation and in his answer during the test, but has the necessary knowledge for correcting these errors by himself;

Assessment “satisfactory (4)” is given to a student who has discovered knowledge of the basic educational program material in the amount necessary for further study and future work in the profession, who while not being sufficiently active in the classroom, has nevertheless independently carried out the main tasks stipulated by the program, learned the main literature but allowed some errors in their implementation and in his answer during the test, but has the necessary knowledge for correcting these errors under the guidance of a teacher;

Assessment “satisfactory (3)” is given to a student who has displayed knowledge of the basic educational program material in the amount necessary for further study and future work in the profession, not showed activity in the classroom, independently fulfilled the main tasks envisaged by the program, but allowed errors in their implementation and in the answer during the test, but possessing necessary knowledge for elimination under the guidance of the teacher of the most essential errors;

Assessment “unsatisfactory (2)” is given to a student who showed gaps in knowledge or lack of knowledge on a significant part of the basic educational program material, who has not performed independently the main tasks demanded by the program, made fundamental errors in the fulfillment of the tasks stipulated by the program, who is not able to continue his studies or start professional activities without additional training in the discipline in question;

Assessment “unsatisfactory (1)” is given to a student when there is no answer (refusal to answer), or when the submitted answer does not correspond at all to the essence of the questions contained in the task.

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

The course is graded at a credit. The questioning starts with a random task assigned to each student and time given for completion of the task. No aids are allowed. The student then proceeds to a chat with the examiner, at which he/she presents his/her solution to the assigned task. The examiner then asks the student several questions that evenly cover the course content. A final grade is assigned based on the quality of answers and demonstrated level of understanding.