Chemoinformatics and Molecular Modelling

Kazan (Volga Region) Federal University

Degree or qualification is awarded: **Master**

Language of study: **Russian**
Mode of study: **full-time**
Duration: **2 years**
Availability of free education: **no**
Price: **180 840 rubles per year**

Programme webpage at the university website:
https://kpfu.ru/eng/academic-units/natural-sciences/alexander-butlerov-institute-of-chemistry

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The purpose of the educational program

The program is aimed at training specialists in chemoinformatics who have knowledge of chemistry, computer science, mathematics and biology, have skills in molecular modeling using various methods, creating and administering databases (including chemical ones). The goal of the program is to develop students' abilities, competencies and skills to navigate in research and production activities related to the development and production of new substances and materials, storage and processing of large volumes of chemical data, to make non-standard, balanced and justified decisions, including those based on data mining.

Why is it worth choosing this program?

The "Chemoinformatics and Molecular Modeling" Master degree program is the first training program in the field of chemoinformatics in the Russian Federation. It is the third active program in the world after the Master's in chemoinformatics at the University of Strasbourg (France) and Indiana University (USA).

This Master's program provides a unique opportunity to gain knowledge at the intersection of sciences, training universal specialists with a wide range of competencies in the application of information technologies, programming and artificial intelligence in solving chemical problems. Our graduates have knowledge in chemistry and biology, design of drugs, materials and reactions, programming, machine learning and data analysis. And in this respect, it can't be compared to any other program in terms of the broad spectrum of the acquired competences.

Another peculiar feature of our program is that our students are able to opt for a double diploma study program: they can take their second year of study at the University of Strasbourg and receive two graduate diplomas - fr om KFU and UniStra. At the same time, it is possible to be trained only at KFU as well.

Description of the educational process

This Master's program was developed in cooperation with the University of Strasbourg.

The study of the theoretical foundations of individual disciplines is always accompanied by practical activities using modern computer tools that have become industry standards. The curriculum consists of two training modules, each lasting one academic year. The first module includes training in programming, selected chapters of advanced mathematics, the basics of quantum chemistry. The purpose of the second module is to teach chemoinformatics, bioinformatics, data mining, molecular dynamics modeling and related disciplines, as well as to prepare a research project (Master's thesis). Every six months the students undergo an internship in scientific laboratories, where they work on real scientific projects in various fields.

Master's students can decide to study on a double degree program: after successful completion of the first year at KFU they have an opportunity to continue their studies at the University of Strasbourg. After successful completion of the

last year, such students receive two diplomas at once - the official graduate diploma of KFU and the equivalent one of the University of Strasbourg.

Skills that students will acquire after completing an educational program

Mastering the program forms a fully skilled specialist in the field of chemoinformatics and molecular modeling, who knows his subject in a sufficiently high degree, is able to learn, can speak foreign languages, is able to make decisions based on a thorough analysis of literature and conduct his own research and be responsible for it, to present himself and his scientific results.

After training, the successful student has programming skills in 2 programming languages, is able to create and manage databases of molecules and chemical reactions, simulate chemical processes using quantum chemistry, predict the properties of molecules and reactions, and perform rational design of molecules, drugs and materials. Considerable attention is paid to communication skills: the ability to make presentations, present scientific reports, give talks at scientific seminars, the ability to work in a team.

Professional Areas Wh ere Graduates Have Advantages

Successful graduates of this program can find jobs in Research & Development departments of pharmacological, oil and chemical industry enterprises, IT-companies engaged in development of new software products for molecular modeling and chemoinformatics, as well as in academic institutions engaged in development of new, practically useful substances. Our graduates have completed post-graduate research programs at KFU and other Russian universities, as well as at the University of Strasbourg (France), University of Oregon (USA), University of Palatsky in Olomouc (Czech Republic), University of Luxembourg, and others. Our collaboration with the BIOCAD biotechnology company gives our students opportunities to undergo internship there, with the prospect of further employment.

The widest range of acquired competencies allows the program graduates to find jobs not only in the professional field - chemoinformatics, quantum chemistry and force field modeling, but also to be in demand in the labor market as programmers, network administrators, chemometrics, statisticians, experts on decision making.

Specializations within this programme