Master Degree Programme COMPUTER MODELING IN PHARMACOLOGY

## Sechenov University and University of Paris

Level: Higher Education- Computer modeling in pharmacology" Master's degree program in 09.04.02 "Information systems and technologies "; **Specialization** : Mathematical and natural sciences;



#### **COMPUTER MODELING IN PHARMACOLOGY**



Students will gain **practical skills** in working with molecular targets, their search and verification

✓ Lectures and practical classes on molecular dynamics will tell about models for constructing energy and conformational landscapes, and their application, when developing new compounds, and when visualizing the mechanism of a particular mechanism of action;



 The applied training technologies and software and hardware of the master's program will allow to work in high-tech pharmaceutical companies in the development and computer modeling departments after graduation.

#### **COMPUTER MODELING IN PHARMACOLOGY**



As a result of study, students will receive the **most up-to-date theoretical knowledge and practical skills** 

- $\checkmark\,$  in the field of molecular modeling of compounds with specified properties;
- ✓ they will learn how to apply and develop tools for predicting the properties of new compounds, such as solubility, toxicity, biological activity, and possible mechanisms of action.

Graduates receive - Master degree Bio-Informatics in the specialty "In silico Drug Design - Macromolecule Modeling" from Université de Paris.

Graduates receive - Master degree in 09.04.02 "Information systems and technologies", specialty "Computer modeling in pharmacology" from Sechenov University.

- we use commercial paid software in our research work and during the study

### **ADVANTAGES / FEATURES OF THE PROGRAM**

There are no more than five universities in Russia that conduct training in such programs. Meanwhile, modern pharmaceutical development and materials science are impossible without computer modeling of new compounds, which is the first stage in the project. The widespread introduction of digital technologies, technologies for working with big data made it possible to use algorithms, software, and machine learning methods in chemistry and materials science.

#### **Goals and objectives:**

Increasing the efficiency and speed of searching for new connections Creating a significant and still unsatisfied demand for specialists in this field.



#### TARGET AUDIENCE

## Graduates of Sechenov University in the following fields of study:

- Graduates of the bachelor's degree in the field of study 06.05.01 "Bioengineering and bioinformatics";
- Graduates of the bachelor's degree in the field of study 19.03.01 "Biotechnology";
- Graduates of the specialist's degree in the field of study 33.05.01 "Pharmacy";
- Graduates of the specialist's degree in the field of study 30.05.01 "Medical Biochemistry";
- Graduates of the specialist's degree in the field of study 30.05.02 "Medical Biophysics";
- Graduates of bachelor's and specialist's degrees from other universities of medical, pharmaceutical, biological, chemical, physical-mathematical and IT profile.



### **ENTRY EXAMINATION**

#### Mathematics

## The form of the entrance test: $\hat{O}$

Computer testing in mathematics

The minimum number of points confirming the successful completion of the entrance test:40 points (out of 100 points)





#### **PRACTICAL TRAINING**

In the leading research organizations of the Russian Federation, large domestic and foreign pharmaceutical companies, structural divisions of Sechenov University (Biomedicine Park, etc.).

## **CURRICULUM**

The curricula of the Russian and French partners of the program are fully coordinated. Therefore, throughout the entire cycle of study in Russia and / or in France, students will take disciplines that can be conditionally divided into three large logical blocks.

#### The curriculum includes the following disciplines:

- UNIX operating systems and the R programming language;
- Fundamentals of biochemistry and biostatistics;
- Programming and mathematical tools (mathematical, programmable, algorithmic);
- Application (practical) and in-depth study (system and ligand biology, databases, toxicology, chemometry);
- Thematic orientation in chemistry and chemoinformatics;
- In-depth study (analysis of big data and biophysical interactions);
- Thematic orientation (protein docking, molecular dynamics, introduction to the computer design of drugs, structural bioinformatics in toxicology);
- Research practice.

- Advanced course in toxicology, biochemistry, chemistry;
- Data analysis in drag design;
- Structural analysis of targets and molecular dynamics;
- High-performance screening: structural and ligandoriented;
- Molecular space analysis;
- Preparation for scientific work in the field of drag design;
- Supervised research work;
- International research practice.

Throughout their studies, students are involved in the scientific agenda of training laboratories and centers, conduct research together with university staff.



## **RESEARCH WORK**

Starting from the first year of study, students begin performing independent research work under the guidance of leading scientistsand specialists of Sechenov University in modern laboratories of the scientific and technological park of biomedicine of Sechenov University, as well as leading research centers in Russia.



едеральное государственное бюджетное учреждение НАЦИОНАЛЬНЫЙ МЕДИЦИНСКИЙ ИССЛЕДОВАТЕЛЬСКИЙ ЦЕНТР КАРДИОЛОГИИ Министерства здравоохранения Российской Федерации



## **RESEARCH WORK**

#### Second year of study at the University of Paris:

Advanced course in toxicology, biochemistry, chemistry; Data analysis in drag design; Structural analysis of targets and molecular dynamics; High-performance screening: structural and ligandoriented; Analysis of molecular space; Preparation for research work in the field of drag design. Supervised research work

introduction to the organization of the research process in the laboratories of the University of Paris;

• performing independent research work, which in the future can serve as the basis for a scientific publication.

The scientific work of undergraduates will be supervised by leading employees of the University of Paris and affiliated research centers.



#### WHERE GRADUATES ARE IN DEMAND

•Local and foreign pharmaceutical companies;

contract organizations;

•research institutes and laboratories engaged in the development of innovative medicines, new materials, conducting research and development in the field of pharmacology, chemistry, materials science, analysis and forecasting in the field of medicine, biology, ecology.



# PARTICIPANCE IN THE MASTER DEGREE PROGRAM WITH THE UNIVERSITY OF PARIS, FRANCE

- 1. The selection of participants to continue their studies at the University of Paris is carried out in the 2nd semester of training by the Joint Coordination Commission;
- 2. Internships and practices in local and foreign pharmaceutical and biotechnological companies;
- 3. 1 or 2 semesters of study in France. A French study visa is issued;
- 4. The level of knowledge of the English language is not lower than B2;

5. The defense of the FQW (Final qualification work) is accepted by a joint SAC (State attestation commission), which includes both employees of the Sechenov University and the University of Paris. According to the results of the defense, the graduate receives diplomas from both universities;

6. Flight, accommodation and other expenses in France provided by student independently;

7. The master's thesis is defended at both universities in turn;

8. Graduates who have successfully mastered the program are awarded state diplomas of Russia and France.



## **PROGRAM DESCRIPTION**

## **Duration of the MODE OF STUDY:** program: two 1 **FULL-TIME** years Language: English 2nd year of study -3 /Russian in France Scholarship at **Students University of Paris** participating in the is possible. program – up to 6

## PARTNER UNIVERSITY - Université de Paris (University of Paris)



**University of Paris** (Université de Paris)

In the Times Higher Education 2020 world rankings of the best universities in the world, the university is ranked 130th, QS WUR 2020 in the field of medicine and life sciences is ranked 70th.

The University of Paris is a leading interdisciplinary university in France, which appeared in 2020 as a result of the merger of 3 famous universities of the French capital: the University of Paris-Diderot, the University of Paris-Descartes and the University of Paris-South.



#### FACULTY

Teaching is conducted mainly by Sechenov University, but employees from companies and institutes of the Russian Academy of Sciences are also involved in the subject of the program.

#### **PROGRAM CURATORS**

#### From the Sechenov University:

Yuri Borisovich Porozov, Head of the Center for Bio-and Chemoinformatics. Institute of Biodesign and Modeling of Complex Systems

#### From the University of Paris:

Anne-Claude Campru, Director of the Computational approaches applied to pharmacological profiling program, in silico drug design

The teaching and management of the FQW (Final qualification work) is carried out by the leading specialists of the Sechenov University and the University of Paris, experts of major research organizations of the Russian Federation.