# INSTITUTIONAL PROFILE: NOVOSIBIRSK INSTITUTE OF ORGANIC CHEMISTRY (NIOCH SB RAS)

### 1. GEOGRAPHICAL POSITION

The region combining North Asia, partly Central Asia, and East Europe is huge and covers more than 10 percent of the Earth's surface. The main part of the region is occupied by the Russian Federation including a large area in the Arctic zone. Approximately two-thirds of the territory of the Russian Federation has not been touched by economic activities and is still an undisturbed environment. In a sense, Novosibirsk is located almost on the border of industrial and pristine parts of Russia and the region as a whole.

Novosibirsk (population more than 1.5 million people) is the most populous city in the Asian part of Russia. It is the administrative center of the Siberian Federal District. Novosibirsk International Airport is the largest beyond the Ural Mountains. It offers numerous direct flights to cities in Europe and Asia.

Akademgorodok is a part of Novosibirsk located 30 km south of the city center. It is the Siberian educational and scientific center surrounded by a birch and pine forest on the shore of the Ob river. Novosibirsk Institute of Organic Chemistry is one of 40 academic research institutes located within Akademgorodok.

### 2. GENERAL AND RELATED INFORMATION

Novosibirsk Institute of Organic Chemistry (NIOCH SB RAS) was founded in 1958 within the framework of the Siberian Branch of the USSR Academy of Sciences. At present, the Institute employs approximately 414 people including 184 researchers (33 professors, 100 researchers with a PhD degree, and 51 graduate students). The Institute is the base for the Department of Organic Chemistry in the Faculty of Natural Sciences, Novosibirsk State University.

### Research departments and labs

- Laboratory of Investigation of Nucleophilic and Radical Ionic Reactions
- Laboratory of Intermediate Products
- Laboratory of Heterocyclic Compounds
- Terpenoid Laboratory
- Laboratory of Nitrogenous Compounds
- Laboratory of Organic Photosensitive Materials
- Laboratory of Halogen Compounds
- <u>Laboratory of Ecological Research and Chromatography</u>
- <u>Laboratory of Physical Methods of Investigation</u>
- Laboratory of Microanalysis
- Laboratory of Pharmacological Investigations
- Laboratory of Biologically Active Compounds
- Laboratory of Medical Chemistry
- Group of Synthesis of Polymerization Catalysts
- Group for Determining Compositions and Structures of Organic Substances
- Metalocomplex Catalysis Group
- Functional Materials Group

## • Organic Electronic Materials Group

The Laboratory of Ecological Research and Chromatographic Analysis, Laboratory of Microanalysis, and Laboratory of Physical Methods of Investigation form a core of the Multi-access Analytical Center. The Analytical Centre was organized in 1987 to support analytical, ecological, and pharmaceutical research.

### 3. THE MAIN ACTIVITIES OF THE ANALITICAL CENTER

The Analytical Centre of NIOCH SB RAS is certified by the Federation Agency on Accreditation. It was ruled that the Centre is able to carry out analysis and identification of organic substances and materials including the analysis of "trace" and "ultra-trace" persistent organic pollutants. The list of the main activities of the Analytical Centre includes

- Targeted analysis and review of environmental objects and identification of pollution sources;
- Development of physicochemical methods for analysis of substances and materials;
- Evaluation of toxicological and pharmacological parameters of substances;
- Independent examination and quality control of food products, cosmetics, soil, water, and air.
- Educational programs on modern analytical methods with hands-on practice with equipment.

The accreditation scope today covers ~350 environmental assays: inorganic and organic, microbiological, ecotoxicological, mutagenicity, and vehicular emission testing and sampling procedures. Concerning persistent organic pollutants (POPs), the following Limits of Quantification Analysis have been certified:

- in water: aldrin, chlordane, chlordecone, dichlorodiphenyltrichloroethane (DDT), dieldrin, endosulfan, endrin, heptachlor, hexachlorobenzene (HCB), gamma-hexachlorocyclohexane (γ-HCH, lindane): 0.00001 mg/l;
- polychlorinated biphenyls (PCBs), polychlorinated dibenzo-p-dioxins (PCDDs), and dibenzofurans (PCDFs): 0.5 pg/l;
- in soil and related sources: aldrin, chlordane, chlordecone, DDT, dieldrin, endosulfan, endrin, heptachlor, hexachlorobenzene (HCB), gamma-hexachlorocyclohexane (γ-HCH, lindane): 0.001 mg/kg;
- polychlorinated biphenyls (PCBs), polychlorinated dibenzo-p-dioxins (PCDDs), and dibenzofurans (PCDFs): 1 ng/kg.

Because of such broad activities in ecological research, NIOCH SB RAS is now considered a reference center for a number of environmental activities. NIOCH SB RAS is the only analytical center in Siberia that can perform the quantitative analysis of ultra-trace amounts of POPs in water, soils, and sediments. NIOCH SB RAS is the only reference institute in Novosibirsk on issues related to water supply and hazardous waste. NIOCH SB RAS currently deals with emergencies in case of disasters, with the police in case of illegal drugs, with the pharmaceutical industry, and so on. It also coordinates the network on soil and groundwater contamination prevention, remediation, and hazardous waste cleanup in Siberia.

### 4. EQUIPMENT AND TECHNICAL PARAMETERS

The Analytical Center is equipped with modem analytical precision equipment allowing for research on analysis of food, biological environments, pharmaceutical drugs, and environmental objects. Equipment of the Center is suitable for research in the fields of ecology, biology, chemistry, and biochemistry at the levels corresponding to modern international standards.

For example, the list of available equipment includes:

- Gas chromatography: MSD, PID, TCD, ECD.
- Chromato-mass-spectrometers: Agilent 6890 with MSD detectors 5973 and 5975
- Liquid chromatography: Detectors: MSD, QTOF, DAD.
- High-resolution mass spectrometer: Thermo DFS
- LC Agilent 1200 Bruker micro-QTOF and others

### 5. ENVIRONMENTAL QUALITY MONITORING

NIOCH SB RAS carries out a variety of environmental monitoring programs, including food, medication, water, and soil quality, encompassing the following areas:

### Expeditions to hidden places of Siberia, Mongolia, and Kazakhstan

Since 1994, NIOCH SB RAS has organized annual expeditions to various off-road regions of Siberia, including Lake Baikal and Buryatia, as well as Mongolia and Kazakhstan. The expeditions were key steps in the implementation of environmental programs including monitoring of POPs: "Environmental safety of Russia," "Protection of the environment and the population from dioxins and dioxinlike toxicants," "Semipalatinsk – Altai," and many others. For further information visit the website http://web.nioch.nsc.ru/leixa/index.htm (in Russian).

The expeditions were aimed at revealing contamination of the Lake Baikal Basin by POPs coming from Mongolia and other surrounding territories. In surface and groundwater, bottom sediments, and bioindicator organisms (bivalve mollusks *Colletopterum*, roach *Rutilus*, pike *Esox lucius*, catfish *Silurus glanis*) have been analyzed for selected POPs.

### **Quality Monitoring**

In Novosibirsk, NIOCH SB RAS is responsible for the licensing of medication. In Siberia and Mongolia, NIOCH SB RAS conducts water quality monitoring programs to assess the quality of aquatic environments for various purposes providing constant testing of the water resources. Since 1994, NIOCH SB RAS has monitored the quality of groundwater by collecting samples at more than 35 sites in Siberia including the region of Lake Baikal. POPs and other substances have been detected and their distribution, possible sources, bioconcentration, and bioaccumulation have been analyzed. The results of these monitoring activities have been published.

NIOCH SB RAS carries out determination of the chemical sediment quality index, related to the aquatic life protection, based on the national permissible levels established for arsenic, heavy metals, and organic compounds. NIOCH SB RAS has also focused on soil condition evaluation on a regional scale.

Some selected results: In 2013, NIOCH SB RAS issued a report presenting data on chromatographic profiles, detailed composition, and current levels of POPs in environmental objects in the basin of the Selenga River and Lake Baikal by the method of chromatography with mass spectrometry. As a result of the analysis of the obtained data, patterns of the intake, distribution, and accumulation of POPs were revealed. The Institute has proven the effectiveness

of the use of data on the qualitative and quantitative POP composition of environmental objects for regional environmental-geochemical and environmental-hygienic assessments of the state of the natural environment and has performed effective detection of sources and zones of strengthening and weakening of the anthropogenic impact on the environment and the development of bioaccumulative POP models for water ecosystems and environmental risk assessment.

In 2015, NIOCH SB RAS published data on the determination of the individual and group composition of low-molecular-mass organic substances of natural and anthropogenic origin according to the analysis of chromatographic profiles and spectral characteristics. The approach enables identification of POPs in the environment of Siberia and Mongolia as well as identification of the main sources of pollution.

### **Chemical emergencies**

Chemical emergencies are unexpected events that may occur during all those activities where hazardous materials are being handled. These events may cause undesirable consequences for public health, for natural resources, and public property. Since 1994, NIOCH SB RAS has worked on the prevention and response to chemical emergencies, providing technical support and intervening in cases involving railroad transport, dangerous substance disposal, industries, petrol plants, and so on.

### SUMMARY concerning NIOCH SB RAS as a new promising Regional Center

- Geographical position (new territories including hidden places of North Asia)
- Experience (25 years) in ecological research
- Highly skilled staff including young scientists
- Available analytical equipment and infrastructure
- Proximity to high-ranking Novosibirsk State University, the Department of Environmental Chemistry
- Experience in research on halogen compounds
- A pilot plant for the development of chemical technology
- Relationships with various ecological laboratories (from Moscow to Vladivostok)
- Proximity (30 km) to downtown Novosibirsk and International Airport

# Organigram of the institution

### The main areas of basic and applied research

Novosibirsk Institute of Organic Chemistry conducts basic and applied research in the following areas:

- studies on the mechanisms of reactions of organic compounds and molecular rearrangements; the structure and properties of compounds and active intermediate species, including the methods for quantum chemical calculations of the structure and properties of compounds;
- methods for synthesizing aromatic, fluoroorganic, heterocyclic, and heteroatomic (containing nitrogen, sulfur, etc.) compounds, including stable radicals, polymers, and monomers;

- development of analytical and instrumental procedures for identifying the structure and configuration of organic compounds and environmental monitoring;
- contributions to solution of environmental problems: identification of environmental contamination; risk assessment and assistance/consultancy on remediation, decontamination of sites/environmental hotspots.
- synthesis and investigation of properties and formation of organic, hybrid, and polymeric materials; development of the basics of the technologies for producing the compounds and agents of practical importance;
- extraction methods and procedures, chemical nature, reactivity, and biological activity of
  plant metabolites. Targeted synthetic transformations and investigation of pharmacological
  properties and the mechanism of action of biologically active agents.

### The Institute today

The Novosibirsk Institute of Organic Chemistry employs 420 people, including 151 researchers (33 Doctors of Science, 96 PhDs, and 20 researchers without an advanced academic degree).

Twenty-two own PhD students and 8 PhD students from other research and educational institutions are currently enrolled in the Institute's PhD program.

The Novosibirsk Institute of Organic Chemistry conducts collaborative research with chemical institutes (the Institute of Organic Chemistry, RAS; the Institute of Organoelement Compounds, RAS; the Ufa Scientific Center, RAS; the Institute of Catalysis, SB RAS; the International Tomography Center, SB RAS; the Institute of Inorganic Chemistry, SB RAS; the Institute of Chemical Biology and Fundamental Medicine, SB RAS; the Irkutsk Institute of Chemistry, SB RAS; and the Institute of Solid State Chemistry and Mechanochemistry, SB RAS), a physics institute (the Institute of Automation and Electrometry, SB RAS), and biological institutes (the Institute of Cytology and Genetics, SB RAS and the State Research Center of Virology and Biotechnology VECTOR), medical research institutes (the Acad. E.N. Meshalkin Novosibirsk Research Institute of Circulation Pathology and the Research Institute of Influenza of the Ministry of Healthcare of the Russian Federation), and state universities (Novosibirsk State University, Novosibirsk State Technical University, Tomsk State University, Krasnovarsk State Pedagogical University, Bashkir State University, Kazan Federal University, and Moscow State University) as well as universities and research laboratories in Belgium, Germany, Japan, Great Britain, the USA, France, Mongolia, Mexico, Estonia, Spain, Kazakhstan, and Belarus within the framework of bi- and multilateral projects and grants.

Individual departments of the Institute are engaged in active collaborations with the leading companies in the USA, Japan, Belgium, Finland, Germany, the Netherlands, Turkey, France, China, South Korea, the Czech Republic, Kazakhstan, and Belarus on a commercial basis.

### Researchers of the Institute annually

- participate in 70–80 projects that are supported by the budget or on a competitive basis, including 7 budget-supported projects, 30–35 Russian Foundation for Basic Research (RFBR) grants, 3–5 Russian Science Foundation grants, 5–6 international projects, grants of the President of Russian Federation, grants from the Administration of the Novosibirsk Region, Novosibirsk City Administration, and UMNIK program grants.

- publish 150–180 research articles and reviews in international and Russian research journals (some of these studies are carried out in collaboration with foreign scientists), 2–5 textbooks, and 2–3 monographs or chapters in multiauthor monographs;
- organize or co-organize 2–4 large research conferences (including schools-conferences for young scientists), and hold 5–10 scientific and educational workshops and presentations;
- deliver over 300 presentations at youth, national, and international conferences;

The research advances at the Novosibirsk Institute of Organic Chemistry have been awarded the Lenin Prize; the State Awards of the USSR, RSFSR, and the Russian Federation; the USSR Council of Ministers Award, the State Prizes of the Russian Federation for young scientists, and a number of diplomas and medals at Russian and international fairs and exhibitions.

The Institute offers the PhD program in the following specialties: Chemistry (organic and physical chemistry) and Basic Medicine (pharmacology and clinical pharmacology). A department for training scientific and pedagogical personnel and the Dissertation Committee awarding academic degrees have been organized. Five to ten doctoral (PhD) and 1–2 Doctor of Science (ScD) dissertations in the field of chemistry are defended each year.

Over 40 employees and PhD students of the Institute are involved in educational activities at schools, colleges (Novosibirsk College of Chemical Technology and etc.), and universities (Novosibirsk State University, Novosibirsk State Pedagogical University, Novosibirsk State Technical University, Novosibirsk State University of Architecture and Civil Engineering); 30–35 employees are academic supervisors of students working on term papers or Bachelor's or Master's theses. At least 30 students enroll in an internship at the Institute; ~10 of those defend their theses and are awarded a Bachelor's, specialist, or Master's degree in chemistry, physics, or biology. The Novosibirsk Institute of Organic Chemistry, SB RAS, serves as the base for the Division of Organic Chemistry (Natural Sciences Department, Novosibirsk State University) and the Division of Chemistry (Department of Natural and Socioeconomic Sciences, Novosibirsk State Pedagogical University).

Tours of the laboratories, the pilot plant, and the museum are organized upon request from schools. The total number of people taking part in these tours annually is more than 300. Researchers working at the Institute deliver popular scientific lectures during the academic year or as part of the Federal or City Days of Science, Science Festivals, or summer science programs (20–30 lectures per year); work as panel members at regional, city, and international middle- and high-school student conferences, organizing committees of the Olympiads on different levels and subjects for middle- and high-school students (the All-Siberian Olympiad, "Future of Siberia," and the All-Russian School Student Olympiad).

# Leadership



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# **Research Departments**

• 1.1 Department of Medical Chemistry

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• 1.2 Department of Physical Organic Chemistry

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### **Multi-access centers**

The **Testing Center** has been established and was certified by the Federal Accreditation Service for technical competence and independence; it now successfully operates on the basis of the Laboratory of Microanalysis, the Laboratory of Physical Methods of Investigation, and the Laboratory of Ecological Research and Chromatographic Analysis.

The Center is equipped with modern high-precision analytical equipment that allows researchers to analyze food and industrial products, biological media, pharmaceuticals, and environmental objects.

The Novosibirsk Institute of Organic Chemistry is the host organization for the Multi-access Chemical Service Center (CSC) uniting the unique and expensive equipment and setups available at chemical institutes of the Novosibirsk Scientific Center. Seven subdivisions have been established as a part of the Center: Departments of Radio Spectroscopy, Optical Spectroscopy, Chromatography with Mass Spectrometry, X-ray Diffraction Analysis and X-ray Spectroscopy, Microanalysis, Toxicological and Pharmacological Analysis, and Research Equipment Maintenance. The equipment available at the Center enables state-of-the-art research in the areas of ecology, biology, chemistry, biochemistry, and medicine that meets modern international standards. The Testing Center is a part of the integrated multi-access centers of the Russian Foundation for Basic Research (RFBR) and the basic-research laboratories of environmental analytical control in the Novosibirsk Region.

The Toxicological and Pharmacological Department performs biological testing of chemical substances, pharmaceuticals, and biologically active food supplements to determine the pharmacological (anti-inflammatory, antiulcer, wound healing, antioxidant, antiarrhythmic, psychotropic, myorelaxant, etc.) activity and toxicity (acute, subchronic, chronic, cumulation, and the allergizing effect).

### Laboratory of Ecological Research and Chromatographic Analysis (LERCA)

Research areas:

Development of the methods for analysis of natural, anthropogenic, and synthetic low-molecular-weight organic compounds, materials, reactions, and processes occurring in living systems and environmental objects.

Investigation of the chemodynamics and the development of bioaccumulation models of persistent organic pollutants for the aquatic ecosystems in the Baikal Natural Area.

Molecular design, synthesis, and studies on the properties of spin-labeled natural biologically active compounds.

### Laboratory of Microanalysis (LMA)

Research areas:

Determining the elemental composition of synthetic and natural compounds and materials of various composition and structure by organic elemental analysis and atomic emission spectroscopy; designing and upgrading the analytical procedures.

Determining the molecular weight of organic compounds and osmolality of solutions by vapor phase osmometry.

Analysis of waste water and workplace air to detect toxic elements and compounds.

### **Center of Spectral Research (CSR)**

Research areas:

Analysis and identification of organic, metal-organic, and inorganic compounds and materials, including nanomaterials with targeted (polymeric, optical, ferromagnetic, and biologically active) properties by molecular spectroscopy for scientific, technological, and medical applications.

The development of physicochemical methods for analysis of substances and materials.

Creation of databases on chromatography with mass spectrometry and on molecular spectroscopy.

Conducting collaborative basic and applied research.

# Laboratory of Pharmacological Research (LPR)

Research areas:

Toxicological and pharmacological examination of plant metabolites and their synthetic derivatives to design original medications.

Studies on the pharmacological properties and the mechanism of action of novel natural and synthetic medicinal products as well as those manufactured by clathration with glycosides and polysaccharides.

Pharmacological screening of novel biologically active natural and synthetic compounds.