

PROCEEDINGS OF THE 2ND INTERNATIONAL CONFERENCE "CHEMISTRY AND BIOLOGICAL ACTIVITY OF OXYGEN- AND SULFUR-CONTAINING HETEROCYCLES" (MOSCOW, OCTOBER 14-17, 2003).

The Second International Conference "Chemistry and Biological Activity of Oxygen- and Sulfur-Containing Heterocycles" in Moscow on October 14-17, 2003, was sponsored by the Russian Academy of the RF President State Service.

The conference organizers were InterBioScreen Ltd. and the charitable fund Scientific Partnership with participation and scientific-logistics support of the Russian Academy of Sciences and OAO Moscow Committee on Science and Technologies of the Moscow Administration.

The chairman of the organizing committee was Prof. V. G. Kartsev. The co-chairmen were Corresponding Member of the Academy of Sciences of Ukraine V. P. Khilya and Corresponding Member of the National Academy of Sciences of the Republic of Kazakhstan S. M. Adekenov.

A total of 73 papers were presented at the conference. The scientific program included world-reknowned scientists, in particular, Prof. Alan Katritzky (University of Florida, USA), Prof. Rolf Huisgen (Munich University, Germany), Prof. Hank van der Plas (Wageningen University, Holland), and Prof. Jan Bergman (Royal Institute of Technology, Organic Chemistry Division, Novum, Sweden). Specialists from other countries, in particular, Belgium, Great Britain, Italy, India, Greece, and Iran, in addition to Russia and CIS countries also participated in the conference.

Nobel laureates Prof. Elias Corey (Harvard University, USA) and Prof. Ryogi Noyori (Nagoya University, Japan) welcomed attendees of the Second International Conference.

The topics of the presentations encompassed a wide range of the chemistry of heterocyclic compounds, including synthesis of novel compounds, development of new methods and approaches to the synthesis of oxygen- and sulfur-containing heterocycles, and the application of calculation methods to the study of physicochemical properties and biological activity of heterocycles and natural compounds. The most representative was a delegation of leading scientists of the Russian Academy of Sciences, in particular, Academicians of the Russian Academy of Sciences (RAS) I. P. Beletskaya, N. S. Zefirov, G. A. Tolstikov, O. N. Chupakhin, and M. G. Voronkov and Professors V. G. Kartsev, M. N. Preobrazhenskaya, L. I. Belen'kii, S. F. Vasilevskii, V. G. Granik, R. G. Kostyanovskii, and others.

The presentation of Prof. A. Katritzky (USA) entitled "Understanding how chemical structure determines physical, chemical and biological properties" included results on the elucidation of the dependence of such properties as melting and boiling points, index of refraction, viscosity, critical concentration for micelle formation, flash point, solvation effects, ability to polymerize, chromatographic, and other properties on molecular weight, number of atoms and bond order and configuration, spatial charge distribution, and polarization effects. The program CODESSA PRO that was developed at the University of Florida can start with a compound structure and predict physicochemical and engineering properties of the compound with a rather high degree of accuracy. This approach will assist in compressing the time required to develop new compounds that are needed in various branches of industry, medicine, and agriculture.

The principal papers by foreign scientists were devoted to classical organic chemistry. For example, Prof. H. van der Plas (Holland) examined new synthetic potentialities of the Chichibabin reaction in his paper "Nucleophiles and azines, a lifelong enjoyment." These can produce nitrogen-, oxygen- and sulfur-containing heterocyclic compounds that potentially have high biological activity.

The paper "Synthesis of sulfur-containing indole derivatives" by Prof. Jan Bergman (Sweden) covered a comprehensive review on results obtained with this class of chemical compounds and information on new ones in addition to new synthetic methods.

Prof. R. Huisgen (Germany) gave the paper "1,3-Dipolar cycloadditions - concertedness: Yes or No?" that demonstrated the enormous synthetic capabilities of 1,3-dipolar cycloaddition reactions and the specifics of the influence of electronic and steric factors on the direction of them.

Among the most interesting plenary talks, that of Academician of the RAS N. S. Zefirov (Moscow), "Computer assisted drug design" should be noted. It examined various methods of computer drug design that enable the first steps in developing a preparation to be shortened to 1-3 years. It discussed new computer-modeling methods developed at Moscow State University and the Institute of Physiologically Active Substances of the RAS that can carry out complex multi-factor structure calculations for compounds with high biological activity using structure—activity relationships.

The paper "Unnatural natural heterocycles. Chemistry and biological activity of unusual oxygen- and sulfur-containing secondary metabolites" of Prof. V. G. Kartsev (Chernogolovka) was devoted to the chemistry of various classes of unusual oxygen- and sulfur-containing natural heterocycles, their biosynthesis, biological activity, and mechanism of action on critical enzyme systems. For example, among 100,000 structures isolated from natural sources such as plants, animals, and marine organisms, practically all contain heterocyclic fragments, in particular, oxygen- and sulfur-containing oxiranes, thiiranes, oxetanes, dithiolanes, di- and trithianes, oxazoles, thiazoles, oxazines, thiazines, oxepines, thiepinines, etc. Heterocyclic compounds with Cl, Br, I, F, B, As, Se, Mo, Fe, Al, and V atoms in their structures have been found in natural sources.

The plenary paper of RAS Academician G. A. Tolstikov (Novosibirsk) "Biologically active higher furanoterpenoids and their derivatives" discussed results from 15 years of studying this class of natural substances. The presence of the furan heterocycle in the higher furanoterpenoids is responsible for the wide range of biological activity exhibited by them, in particular, antitumor, antiviral, antibacterial, etc. Lambertianic acid, which is isolated from pine nuts, and the synthesis of derivatives containing a furan ring are studied at the Novosibirsk Institute of Organic Chemistry.

RAS Academician O. N. Chupakhin (Ekaterinburg) gave a paper entitled "Synthesis and transformation of fluorine-containing chromones" that explored the chemistry of chromones, in particular, the preparation of fluorine-containing biologically active compounds in this series. Methods were developed for preparing 2-alkoxycarbonyl(carboxy)-5,6,7,8-tetrafluorochromones and studying their transformation pathways. The mechanisms and certain aspects of the chemo- and stereoselectivity of the involved reactions were discussed in detail.

The paper of Prof. V. G. Granik (Moscow), "Oxygen- and sulfur-containing heterocyclic compounds - NO donors and NO-synthase inhibitors," reviewed data from the last 15 years on oxygen- and sulfur-containing heterocyclic compounds exhibiting NO-donor activity and acting as NO-synthase inhibitors. Research on known medicinal compounds was discussed. It has been found that nitrogen donors occur among many of these. The need for more attentive examination of the contribution of NO generation to the mechanism of medicinal activity and the possible revision of ingrained concepts of these mechanisms were pointed out.

Among the most interesting presentations was that of Prof. R. G. Kostyanovskii (Moscow), "Story of the dilactones of N. D. Zelinskii," concerning the study of the Zelinskii reaction, improvement and development of methods for inducing auto-assembly of complicated molecules containing a lactone ring from simpler ones through the minimal number of steps.

The review of Prof. V. P. Khilya (Kiev) entitled "Functionally modified flavonoids, isoflavonoids, coumarins, and heterocyclic systems based on them" discussed research results on the synthesis and properties of flavonoids, isoflavonoids, and their heterocyclic analogs. He presented information on the optimization of methods for preparing 3-hetarylchromones and certain heterocyclic analogs and flavone and coumarin derivatives, synthetic methods for glycosides of isoflavones, stereochemical features of modified flavonoids and isoflavonoids, systematic investigation of the chemical and biological properties of modified flavonoids, and the identification among them of new highly effective medicinal preparations. The functionalization of these compounds by such pharmacophores as amino acids, oligopeptides, carboxylic acids, amines, carbohydrates, five- and six-membered heterocycles, and arenes was also examined.

A. L. Mikhal'chuk from the school of Academician A. A. Akhrem (Minsk, Belarus) presented a paper on the reactivity of heterocyclic β,β' -tricarboxyl compounds and their anions.

The Institute of the Chemistry of Plant Substances of the Academy of Sciences of the Republic of Uzbekistan (Tashkent, Uzbekistan) was represented by the paper of I. D. Sham'yanov and Kh. M. Shakhidoyatov on sesquiterpene lactones of Central Asia.

A plenary lecture by Corresponding Member of the National Academy of Sciences of the Republic of Kazakhstan S. M. Adekenov, Candidate of Chemical Sciences A. T. Kulyasov (Institute of Phytochemistry of the Ministry of Education and Science of the Republic of Kazakhstan [MES RK]) entitled "Sesquiterpenoids in the synthesis of lactone derivatives," and

oral presentations by Corresponding Member K. D. Praliev and Candidate of Chemical Sciences V. K. Yu (Institute of Chemical Sciences) entitled "Hetero(thia-, oxa-)cycles with the N-alkoxyalkylpiperidine fragment" and by Prof. K. B. Erzhanov and Candidate of Chemical Sciences S. A. Vizer (Al-Farabi Kazakh National Institute) entitled "Synthesis of heterocycles via catalytic intramolecular cyclization and carbonylation of acetylenic compounds" were contributed from the Republic of Kazakhstan. Poster presentations by young scientists A. N. Talzhanov ("Chemical modification of the guaianolide austricin") and V. I. Yamovii ("Crystal structures of pinostrobin oxime and its chlorination product in methanol") were contributed from the Institute of Phytochemistry of the MES RK.

The Second International Conference "Chemistry and Biological Activity of Oxygen- and Sulfur-Containing Heterocycles" reached a high level that provides hope that new scientific bonds and contacts will be formed, the chemistry of heterocyclic compounds will be further developed, and the scientific collaboration and partnership of scientists from various countries will be strengthened.

Leading scientists from the former Soviet Union working on the chemistry of heterocyclic compounds, bioorganic chemistry, and the chemistry of natural compounds participated in the conference.

Chief Scientific Secretary of the National
Center for Biotechnology of the Republic
of Kazakhstan, Candidate of Chemical
Sciences A. T. Kulyasov
Republic of Kazakhstan, Astana