Dedicated to the memory of Nikolay Serafimovich Zefirov (1935–2017)

An oak is a tree.
A deer is an animal.
Russia is our fatherland.
Death is inevitable.
A good idea is forever.

After Vladimir Nabokov

Nicolay Serafimovich occupies a special place in my heart, and he will be there until it stops beating. This volume is a small tribute to his memory, which hopefully would not be the last. After all, the authors of this volume take a time from their busy lives to create their contributions. Among them are young researches who never met Nikolay Serafimovich in person – a clear sign of his lasting influence. In this respect, it is prudent to note that the history of science is not only the history of researches, but also the history of ideas. Of course, these ideas should be good enough to ensure their own survival and propagation. Having this in mind, the current special volume collection could serve as a reflection of this notion.

It would probably be naïve to think that Nikolay Serafimovich invented all the ideas presented in the special volume. Good ideas almost always have many fathers. Any individual contribution therefore could be judge from the perspective of early realization and endorsement. Nikolay Serafimovich was never shy of new ideas. Last, but least, even good ideas require people behind them. Nikolay Serafimovich was always surrounded by capable and creative scientists. Not surprisingly, Nikolay Serafimovich research portfolio is very diverse. Due to the scope limitations of the current volume, only a few ideas from his vast research portfolio will be highlighted here.

This special volume features a mini-review of Mekhman S. Yusubov and Viktor V. Zhdankin, "Zefirov's reagent and related hypervalent iodine triflates". The mini-review is devoted to iodonium reagents, one of which bears Zefirov's name. The main ideas behind this research were actually developed in the late-1980s within the framework of so-called "hypervalent" compounds – *d*-element molecules formally violating 8-electrons

rule. These, for example, include xenon compounds, but, so far, only iodonium reagents achieved widespread use in organic synthesis.

Not only synthetic organic chemistry, but also computational methods were of interest for Nikolay Serafimovich. He early on recognized the importance of computers in chemistry, and was a visionary, a pioneer and a major founder of the computational lab at Zelinsky Institute of Organic Chemistry. In the 1980s it was a bold step, taking into account the state of computer development in general and in the Soviet Union in particular. This initiative supported not only traditional *ab initio* and semi-empirical calculations, but also early AI research in chemistry in the 1990s and beyond. This effort is represented in this special issue by several papers. One of these papers, "Structure and complexation energy of benzotrifuroxan–benzene molecular complex", is written by Dmitry V. Khakimov, Ivan D. Nesterov and Tatyana S. Pivina. In this paper, the authors use a combination of quantum chemistry and atom–atom potentials methods to develop a technique for modeling the structure and estimating the complexation energy of a binary organic complex in gas and crystal phases, which is exemplified by benzotrifuroxan–benzene molecular complex. Another paper, "Introducing LibXC into GAMESS (US)" by Igor S. Gerasimov, Federico Zahariev, Sarom S. Leang, Anton Tesliuk, Mark S. Gordon and Michael G. Medvedev, presents the interface between LibXC and GAMESS (US), which allows calculations with density functional approximations, such as r2SCAN, M06-SX and CAM-QTP00. Finally, the paper entitled "Conformational effects of 1,5,9-substitution in symmetric bicyclo[3.3.1]nonane analogues" by Sergey A. Pisarev and Vladimir A. Palyulin reports the high-level *ab initio* calculations on several derivatives of bicyclo[3.3.1]nonane, 1-aza- and 1,5-diazabicyclo[3.3.1]-nonanes.

Fundamental changes in Russia after the 1991 revolution brought inevitable changes in science as well. Self-sustainability of scientific enterprise became an urgent need. Even in these tough times, Nikolay Serafimovich continued the research unabated, using a network of his international friends, and a dive into medicinal chemistry. Two excellent papers form his longtime friends and colleagues, "Academician N. S. Zefirov, his life and accomplishments" by Peter J. Stang and "In memory of Nikolay Serafimovich Zefirov" by Armin de Meijere, could serve as a proof of these deep connections within the international science enterprise. As for medicinal chemistry, the papers presented in this

volume prove the validity of the chosen direction. One of the papers, "Reverse fragment based drug discovery approach via simple estimation of fragment contributions" by Dmitry A. Shulga, Nikita N. Ivanov and Vladimir A. Palyulin, is actually a cross-field contribution in both computational and medicinal chemistry. It presents a reversed fragment based drug discovery (R-FBDD) approach for prediction of the binding/activity of a drug candidate to a specified target. Another paper, "*N*-(4-Methoxyphenyl)-substituted bicyclic isothioureas: effect on morphology of cancer cells" by Anna V. Evdokimova, Alexander A. Alexeev, Evgeniya V. Nurieva, Elena R. Milaeva, Sergei A. Kuznetsov and Olga N. Zefirova, regarding induced changes in the morphology of human lung carcinoma cells A549, which do not affect the microtubule net, is written in more traditional medicinal chemistry venue. In another paper, "Novel conjugates of 4-amino-2,3-polymethylenequinolines and vanillin as potential multitarget agents for AD treatment" by Galina F. Makhaeva, Igor V. Serkov, Nadezhda V. Kovaleva, Elena V. Rudakova, Natalia P. Boltneva, Ekaterina A. Kochetkova, Alexey N. Proshin and Sergey O. Bachurin, the authors explore a series of novel conjugates of 4-amino-2,3-polymethylene quinolines with phenolic antioxidant vanillin, which inhibit AChE and BChE, and displace propidium from the PAS AChE. Finally, the paper "Synthesis of modified conformationally fixed tricarbocyanine dyes for conjugation with therapeutic agents" by Irina A. Doroshenko, Kamilla G. Aminulla, Viatcheslav N. Azev, Tatiana M. Kulinich, Vladislav A. Vasilichin, Alexander A. Shtil and Tatyana A. Podrugina, reports novel β-alanine modified tricarbocyanines containing two sulfonate groups with total negative charge of the fluorophore for bioimaging applications.

The impact of Nikolay Serafimovich vision in science extends well beyond these examples. His uninhibited scientific curiosity and willingness to entertain cool ideas from all parts of chemistry serve as an inspiration for many of his colleagues and students, including myself. "Pulsed aluminum battery" presented in this issue could serve as an illustration of this point.

As a conclusion, "classic" organic chemistry was always bread-and-butter of Zefirov's group research. Several papers in this area from close collaborators and long-term members of Zefirov's group are presented in this issue. While not at all comprehensive, these papers demonstrate the breadth and agility of this scientific endeavor. One of these

papers, "Direct oxidative functionalization of saturated dispiro-cyclopropanated bicyclo[3.3.1]nonanes" by Kristian S. Andriasov, Kseniya N. Sedenkova, Marina G. Eremenko, Igor P. Gloriosov, Yuri K. Grishin, Tamara S. Kuznetsova and Elena B. Averina, is devoted to the oxidative chemistry of dispiro[cyclopropane-1,3'-bicyclo[3.3.1]nonane-7′,1″-cyclopropanes]. It can be linked to the vast research effort in the area of strained molecules, including molecular landmarks - triangulanes. In another paper, "Synthesis, coordination and extraction properties of 2,3-bis(diphenylphosphoryl)pyridine toward f-block elements" by Oleg I. Artyushin, Anna V. Vologzhanina, Aleksandr N. Turanov, Vasilii K. Karandashev and Valery K. Brel, the authors report the synthesis of 2,3-bis(diphenylphosphoryl)pyridine, a novel N,O-donor bidentate organophosphorus ligand, which can serve as an efficient extractant for recovery of f-block elements from nitric acid solutions. Another paper, "A new P-heterocyclic type of phosphonium–iodonium ylides based on dibenzophosphole" by Anton S. Nenashev, Dmitry A. Dospekhov and Tatyana A. Podrugina, reports a novel mixed phosphonium–iodonium ylide, which was synthesized by alkylation of 5-phenyl-5H-dibenzophosphole with phenacyl bromide followed by deprotonation and oxidation of the resulting phosphonium ylide with (diacetoxyiodo)- benzene. Finally, two papers in this volume are related to the use of NMR, in combination with computational tools, for evaluation of molecular structure conformations and signal assignments. One of these papers, "Conformational energy (A-value) of the 4-phenyl-1,2,3-triazolyl group" by Mulinde R. Ruyonga and Vyacheslav V. Samoshin, reports conformational energy (A-value) of the 4-phenyl-1,2,3- triazolyl group in a set of (4-phenyl-1,2,3-triazol-1-yl)cyclohexanes. In another paper, "Structure revision of ent-kaurane diterpenoids, isoserrins A, B, and D, enabled by DU8+ computation of their NMR spectral data" by Ivan M. Novitskiy, Tina A. Holt and Andrei G. Kutateladze, the authors report the correct assignments of ^{13}C NMR peaks and structure revisions in isoserrins A, B, and D, which were recently isolated from medicinal plant Isodon serra.

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