

ANNIVERSARIES AND DATES



NIKOLAI SERAFIMOVICH ZEFIROV
(on his 75th jubilee)

Outstanding scientist in the fields of organic, mathematical, and medicinal chemistry, Nikolai Serafimovich Zefirov was born on 13 September 1935 in Yroslavl. In 1958 he graduated from the Faculty of Chemistry of M.V. Lomonosov Moscow State University with a "Red Diploma". He became Doctor of Chemical Science (1966), Professor (1973) and head of Chair of Organic Chemistry, Faculty of Chemistry of the Moscow State University (from 1993 to the present), corresponding member of the Russian Academy of Sciences (1981), and Academician of the Russian Academy of Sciences (1987). N. S. Zefirov – Academician of the International Academy of Mathematical Chemistry, Academician of the International Academy of Informatization, Academician of the Russian Academy of Natural Sciences, member of the International Academy on the Uses of Iodine, honored Professor of the M. V. Lomonosov Moscow State University, honorary Professor of a number of leading universities of Europe and the USA, honorary Academician of the Academy of Sciences of the Republic of Bashkortostan. N. S. Zefirov has been awarded state orders and medals, he was conferred with the State Prize of the USSR, Prize of the Government of the Russian Federation in Science and Technology (2002), the Butlerov and Lomonosov prizes, and others. For many years N. S. Zefirov was the director and is currently the scientific leader of the Institute of Physiologically Active Compounds of the Russian Academy of Sciences.

Academician N. S. Zefirov, an acknowledged leader in organic and mathematical chemistry, is one of the most cited chemists. His contribution in the development of organic synthesis is difficult to overestimate: the discovery of a series of new electrophilic addition reactions, new classes of organic compounds

Translated from *Khimiya Geterotsiklicheskikh Soedinenii*, No. 9, pp. 1283-1294, September, 2010.

(triangulanes, organic perchlorates, heteroadamantanes, etc.), new unique reagents (hypervalent compounds of iodine, selenium, and tellurium, nitrosulfates, etc.), and the discovery of new phenomena of the nucleophilicity of nucleofugal anions. N. S. Zefirov founded the Russian school of mathematical chemistry and computation of molecular design. He developed methods of mathematical chemistry in applications to problems of medicinal chemistry which allowed the development of molecular modeling of receptors of humans and the planning of the synthesis of innovative medicinals of a new generation. In recent years he has developed the synthesis of new classes of heterocycles, strained polycyclopropane structures, the synthesis of essentially new reagents, for example polynitromethanes for the synthesis of nitro-substituted heterocycles, discovered universal catalysts for a series of processes, new rearrangements, developed the concept of molecular similarity for the prognosis of properties of chemical compounds and for molecular modelling of receptors of the central nervous system of man, for example modelling the open and closed forms of the GABA_A receptor and the mechanism of its activation, the creation of mathematical apparatus to survey structures with previously targeted properties, carried out the synthesis of compounds possessing antitumor activity, developed a method for the synthesis of phosphorus-containing oligopeptides, synthesis of polyspirocyclic amino acids of the cyclopropane series, pseudo- γ -glutamylpeptides, studied the immediate and delayed neurotoxicity in a series phosphorylated oximes, created allosteric modulators of the AMRA-receptor, pharmacologically active 3,7-diazabicyclo[3.3.1]nonanes, hydrogenated pyrido(4,3-*b*)indoles, improved cognitive functions and memory, developed new antineoplastics with proapoptotic properties, etc.

N. S. Zefirov is the initiator of the study of medicinal chemistry in Russia and created the new specialty of "Medicinal Chemistry" in the Faculty of Chemistry of Moscow State University .

In the chemical schools of Academic N. S. Zefirov in the Moscow State University and in Institute of Physiologically Active Compounds of the Russian Academy of Science more than one hundred Candidates and more the 20 Doctoral Dissertations have been submitted.

N. S. Zefirov has published more than 1600 scientific papers and has obtained more than 100 author's certificates and patents.

In parallel with his scientific and pedagogical activities, N. S. Zefirov was active in science organizing work. For many years he chaired scientific and dissertation committees, commissions and sections of the Russian Academy of Sciences, the D. I. Mendeleev Russian Chemical Society, departments of ministries, etc. An international sign of the respect of N. S. Zefirov is shown in that he is member of the editorial boards of the most prestigious journals: *Tetrahedron Asymmetry*, *Chemical Information and Comput. Sci.*, *Sulfur Reports*, *Sulfur Letters*, *Current Topics in Medical Chemistry*, *Khimiya Geterotsiklicheskikh Soedinenii (Chemistry of Heterocyclic Compounds)*, etc.

Nikolai Serafimovich is an inventive, learned, friendly and sympathetic essential scientist who enjoys deep esteem, love and authority

In his 75th year Nikolai Serafimovich Zefirov continues to be active, filled with creative work, and is a model and example for scientists, co-workers, and colleagues.

For many years Nikolai Serafimovich was a member of the editorial board of our journal, presently a member of the advisory board, and he and his co-workers are regularly among our authors.

We heartily congratulate Nikolai Serafimovich on jubilee and wish him new creative successes and achievements, new ideas and their implementation, successful completion of intentions, selfless co-workers and disciples, prolonged strong health, happy years of life and we hope that he will continue as our co-worker.

The Editorial Board

A Listing of the Main Publications of Academician of the Russian Academy of Sciences N. S. Zefirov for the Period 2006-2010.

1. V. I. Chupakhin, V. A. Palyulin, and N. S. Zefirov, Modeling the open and closed forms of GABA_A receptor: Analysis of ligand-receptor interactions for the GABA-binding site, *Dokl. Biochem. Biophys.*, **408**, 169-174 (2006).
2. E. B. Averina, R. R. Karimov, K. N. Sedenkova, Yu. K. Grishin, T. S. Kuznetsova, and N. S. Zefirov, Carbenoid rearrangement of *gem*-dihalospiropentanes, *Tetrahedron*, **62**, 8814-8821 (2006).
3. E. V. Averina, N. N. Yashin, Yu. K. Grishin, T. S. Kuznetsova, and N. S. Zefirov, Synthesis of (\pm)-(2-methylenecyclopropyl)glycine and (\pm)-4-[amino(carboxymethyl)]spiro[2.2]pentane-1-carboxylic acid, *Synthesis*, 880-884 (2006).
4. R. A. Gazzaeva, A. N. Fedotov, E. V. Trofimova, O. A. Popova, S. S. Mochalov, N. S. Zefirov, Synthesis of *o*-nitrosoacylbenzenes from *o*-nitrobenzyl alcohols and their derivatives, *Russ. J. Org. Chem.*, **42**, 87-99 (2006).
5. E. M. Budynina, O. A. Ivanova, E. V. Averina, T. S. Kuznetsova, and N. S. Zefirov, Ring opening of 1,1-dinitrocyclopropane by addition of C, N, O, and S nucleophiles, *Tetrahedron Lett.*, **47**, 647-649 (2006).
6. A. N. Zakharov and N. S. Zefirov, Catalytic properties of mono- and oligomeric Cu(II) phenylhydrazone imine chelates immobilized on zeolite with a topological anchor, *Russ. J. Gen. Chem.*, **76**, 1353-1362 (2006).
7. N. V. Zyk, A. Yu. Gavrilova, O. A. Mukhina, O. B. Bondarenko, and N. S. Zefirov, Sulfenic acid esters as promising sulfenylating agents, *Russ. J. Org. Chem.*, **42**, 1856-1857 (2006)
8. N. V. Zyk, A. Yu. Gavrilova, O. A. Mukhina, O. B. Bondarenko and N. S. Zefirov, Halo(trimethyl)silanes as activating coreagents in sulfenylation of olefins, *Russ. Chem. Bull., Int. Ed.* **55**, 1865-1866 (2006).
9. E. V. Radchenko, V. A. Palyulin, and N. S. Zefirov, Local molecular characteristics in quantitative analysis of "structure-activity" relationships, *Ross. Khim. Zh.*, **100** (2), 76-85 (2006).
10. A. V. Ivanov, P. A. Svinareva, I. V. Zhukov, L. G. Tomilova, and N. S. Zefirov, New diphthalocyanine complexes of rare-earth metals based on 4,5-isopropylidenedioxyphthalonitrile, *Russ. Chem. Bull., Int. Ed.*, **55**, 281-286 (2006).
11. V. V. Kalashnikov, L. G. Tomilova, and N. S. Zefirov, A convenient route to 9,10-dicyano-1,2,3,4,5,6,7,8-octahydrophenanthrene, *Russ. J. Gen. Chem.*, **76**, 329-330 (2006).
12. M. I. Lavrov, V. A. Palyulin, and N. S. Zefirov, Design and synthesis of allosteric modulators of AMPA receptors, in: *Proc. of XIII Russian National Congress "Man & Drug", Moscow, Russia, April 3-7 [in Russian]*, 24, (2006).
13. O. A. Ivanova, E. M. Budynina, E. V. Averina, T. S. Kuznetsova, and N. S. Zefirov, Application of a thermal β -elimination reaction to N-alkoxy-3,3-dinitroisoxazolidines: Synthesis of 3-nitroisoxazolines, *Synthesis*, 706-710 (2006).
14. E. D. Matveeva, T. A. Podrugina, M. V. Prisyajnoy, and N. S. Zefirov, Ketones in catalytic three-component "one-pot" Kabachnik-Fields synthesis of α -amino phosphonates, *Russ. Chem. Bul., Int.Ed.*, **55**, 1209 (2006).
15. E. D. Matveeva and N. S. Zefirov, Amino acids in a three-component synthesis of alpha-aminophosphonates derivatives, *Russ. J. Org. Chem.*, **42**, 1237-1238 (2006).
16. S. S. Mochalov, P. I. Gadzhieva, N. S. Zefirov, T. A. Voronina, L. N. Nerobkova, T. A. Gudasheva, 6-(4'-Chlorobenzoyl)-7-(N-4"-nitrobenzoyl)amino-1,4-benzodioxane and their analogs possessing anticonvulsive activity, Russ. Pat. 2277091 (2006).

17. E. D. Matveeva, M. V. Proskurnina, and N. S. Zefirov, Polyvalent iodine in organic chemistry: recent developments, 2002-2006, *Heteroat. Chem.*, **17**, 595-617 (2006).
18. M. I. Skvortsova, I. V. Stankevich, V. A. Palyulin, and N. S. Zefirov, Molecular similarity concept and its use for predicting the properties of chemical compounds, *Russ. Chem. Rev.*, **75**, 961-979 (2006).
19. Yu. V. Skornyakov, M. V. Proskurnina, and N. S. Zefirov, Synthesis of cyclopropenes, in: *Advances in Organic Catalysis and the Chemistry of Heterocycles [in Russian]*, Khimiya, Moscow, 141-168 (2006)
20. A. Yu. Tolbin, V. E. Pushkarev, L. G. Tomilova and N. S. Zefirov, Synthesis and spectral properties of new planar binuclear phthalocyanines sharing the benzene ring. *Russ. Chem. Bull., Int. Ed.*, **55**, 1155-1158 (2006).
21. D. A. Shulga, A. A. Oliferenko, S. A. Pisarev, V. A. Palyulin, and N. S. Zefirov, Modelling of atomic RESP charges with the use of topological calculation schemes. *Dokl. Chem.*, **408** (1), 76-80 (2006).
22. A. Yu. Tolbin, V. E. Pushkarev, L. G. Tomilova, and N. S. Zefirov, Preparation and spectral properties of new planar binuclear phthalocyanine sharing one benzene ring, *J. Porphyrins Phthalocyanines*, **10**, 900 (2006).
23. L. G. Tomilova, A. Yu. Tolbin, V. E. Pushkarev, M. O. Breusova, and N. S. Zefirov, Synthesis and investigation of new phthalocyanines and their analogues, *J. Porphyrins Phthalocyanines*, **10**, 516 (2006).
24. S. S. Tratch, M. S. Molchanova, and N. S. Zefirov, New approaches to degenerate interconversions of organic structures. 1. Levels of structural degeneracy and computer-aided search for degenerate rearrangements, *Croat. Chem. Acta*, **79**, 339-353 (2006).
25. N. V. Yashin, E. V. Averina, Yu. K. Grishin, T. S. Kuznetsova, and N. S. Zefirov, Reduction of 1-nitrospiro[2.2]pentanecarboxylates: Convenient synthesis of novel polyspirocyclic cyclopropane amino acids, *Synthesis*, 279-284 (2006).
26. N. S. Zefirov and V. A. Palyulin, Quantitative description of ring shape and its application in conformational analysis, in: *Abstr. IV National Conf. Crystallochemistry, Chernogolovka, Russia [in Russian]*, II-9, (2006).
27. I. I. Baskin, V. A. Palyulin, and N. S. Zefirov, Monolayer perseptrones in the study of "structure-activity" relationships of organic compounds, *Ros. Khim. Zh.*, **100** (2), 86-96 (2007).
28. R. L. Antipin, E. K. Beloglazkina, N. V. Zyk, and N. S. Zefirov, Arylselenation of conjugated dienes by arylselenamides in the presence of phosphorous (V) oxyhalides, *Tetrahedron Lett.*, **48**, 729-731 (2007).
29. T. Yu. Baranova, O. N. Zefirova, N. V. Averina, V. V. Boyarskikh, G. S. Borisova, N. V. Zyk, and N. S. Zefirov, Synthetic approach to preparation of indole derivatives fused with a bicyclo[3.3.1]nonane framework, *Russ. J. Org. Chem.*, **43**, 1196-1201 (2007).
30. A. E. Voronkov, I. I. Baskin, V. A. Palyulin, and N. S. Zefirov, Molecular modelling of the complex between the XWNT8 protein and the CRD domain of the MFZD8 receptor, *Dokl. Biochem. Biophys.*, **412** (1), 8-11 (2007).
31. R. A. Gazzaeva, M. I. Khasanov, S. S. Mochalov, and N. S. Zefirov, 4H-3,1-Benzoxazines from *o*-aminoacylbenzenes, *Khim. Geterotsikl. Soed.*, 941-954 (2007). [*Chem. Heterocycl. Comp.*, **43**, 799-810 (2007)].
32. N. I. Zhokhova, V. A. Palyulin, I. I. Baskin, A. N. Zefirov, and N. S. Zefirov, Fragmental descriptors in the QSPR method: Their use for calculating the enthalpies of vaporization of organic substances. *Russ. J. Phys. Chem., A*, **81**, 9-12 (2007).
33. N. I. Zhokhova, V. A. Palyulin, I. I. Baskin, A. N. Zefirov, and N. S. Zefirov, Fragmental descriptors with labeled atoms and their application in QSAR/QSPR studies, *Doklady Chemistry*, **417** (2), 282-284 (2007).

34. O. N. Zefirova, A. G. Diikov, N. V. Zyk, and N. S. Zefirov, O. N. Zefirova, A. G. Diikov, N. V. Zyk, and N. S. Zefirov, Ligands of the colchicine site of tubulin: a common pharmacophore and new structural classes. *Russ. Chem. Bull., Int. Ed.*, **56**, 680–688 (2007).
35. A. A. Ivanova, I. I. Baskin, V. A. Palyulin, and N. S. Zefirov, Estimation of ionization constants for different classes of organic compounds with the use of the fragmental approach to the search of structure-property relationships, *Dokl. Chem.*, **413** (2), 90-94 (2007).
36. A. A. Kravtsov, P. V. Karpov, I. I. Baskin, V. A. Palyulin, and N. S. Zefirov, "Bimolecular" QSPR: Estimation of the solvation free energy of organic molecules in different solvents, *Dokl. Chem.*, **414** (1), 128-131 (2007).
37. R. Gleiter, D. B. Werz, F. Rominger, E. V. Zhutov, N. S. Zefirov, and M. V. Proskurnina, Insight into the molecular structure and reactivity of α,ω -dialkoxy-substituted ethyne and butadiyne, *Eur. J. Org. Chem.*, 5834-5839 (2007).
38. A. A. Ivanov, V. A Palyulin, and N. S. Zefirov, Computer aided comparative analysis of the binding modes of the adenosine receptor agonists for all known subtypes of adenosine receptors, *J. Mol. Graphics Modell.*, **25**, 740-754 (2007).
39. O. A Ivanova, E. M. Budynina. E. B. Averina, T. S. Kuznetsova, V. A. Palyulin, and N. S. Zefirov, [3+2] Cycloaddition of diazocarbonyl compounds to 1,1-dinitroethenes: Synthesis of functionalized *gem*-dinitrocyclopropanes, *Synthesis*, 2009-2013 (2007).
40. E. D. Matveeva, T. A. Podrugina, M. V. Prisyazhnoi, I. N. Rusetskaya, and N. S. Zefirov, Three-component catalytic method for synthesis of phosphonates with the α -amino acids as amine component, *Russ. Chem. Bull., Int. Ed.*, **56**, 798-805 (2007).
41. E. D. Matveeva, T. A. Podrugina, Yu. K. Grishin, A. S. Pavlova, and N. S. Zefirov, Phosphonium-iodonium ylides in nucleophilic substitution reactions, *Russ. J. Org. Chem.*, **43**, 201-206, (2007).
42. D. I. Osolodkin, V. I. Chupakhin, V. A. Palyulin, and N. S. Zefirov, Modelling and analysis of ligand-receptor interactions in the GABA_A receptor. *Dokl. Biochem. Biophys.*, **412**, 25-28 (2007).
43. V. A. Palyulin, E. V. Radchenko, I. I. Baskin, and N. S. Zefirov, Prediction of drug selectivity, in: *Proc. of the XIV Russian National Congress "Man & Drug", Moscow, Russia* [in Russian], 309 (2007).
44. A. A. Melnikov, V. A. Palyulin, and N. S. Zefirov, Generation of molecular graphs for QSAR studies: An approach based on supergraphs, *J. Chem. Inf. Model.*, **47**, 2077-2088 (2007).
45. A. Yu. Tolbin, L. G. Tomilova, and N. S. Zefirov, Non-symmetrically substituted phthalocyanines: synthesis and structure modification. *Russ. Chem. Rev.*, **76**, 681-692 (2007).
46. O. N. Zefirova, K. A. Potekhin, A. I. Touchin, N. V. Averina, T. Yu. Baranova, N. V. Zyk, and N. S. Zefirov, Molecular and crystal structure of indole derivatives fused with substituted bicyclo[3.3.1]nonane, *Struct. Chem.*, **18**, 457-460 (2007).
47. O. N. Zefirova, L. A. Zasurskaya, E. V. Nurieva, V. V. Zyk, and N. S. Zefirov, Molecular and crystal structure of the ethylene acetal of *endo-endo*-3-trityloxymethylbicyclo[3.3.1]nonan-2-on-7-ol, *Struct. Chem.*, **18**, 461-464 (2007).
48. O. N. Zefirova, E. V. Nurieva, V. N. Nuriev, K. A. Potekhin, A. V. Maleev, N. V. Zyk, and N. S. Zefirov, Crystal structure of the tritiated product of 3-hydroxymethylbicyclo[3.3.1]nonan-2-on-7-ol ethylene acetal cyclization, *Mendeleev Commun.*, **17**, 332-334 (2007).
49. A. V. Chemagin, N. V. Yashin, E. B. Averina, T. S. Kuznetsova, and N. S. Zefirov, New method for the synthesis of 1-aminospiro[2.2]pentane-1,4-dicarboxylic acid, *Dokl. Chem.*, **419** (2), 113-115 (2008).
50. S. O. Bachurin, V. V. Grigor'ev, N. S. Zefirov, M. I. Lavrov, V. L. Lapteva, and V. A. Palyulin, N,N'-substituted 3,7- diazabicyclo [3.3.1]nonanes, with pharmacological effect, pharmacological composition on their base, and application method, Russ. Pat. 2333211 (2008).

51. S. O. Bachurin, S. I. Gavrilova, V. V. Grigor'ev, B. K. Beznosko, and N. S. Zefirov, Means for improvement of cognitive functions and memory on the basis of hydrated pyrido[4,3-*b*]indoles (variants), pharmacological means on their basis and method of its application, Russ. Pat. 02334514 (2008).
52. O. B. Bondarenko, A. Yu. Gavrilova, L. G. Saginova, N. V. Zyk, and N. S. Zefirov, New aspects of nitrosation of arylcyclopropanes: Nitrosation of phenylcyclopropanes with bulky alkyl substituents in the small ring, *Khim. Geterotsikl. Soed.*, 1566-1575 (2008). [*Chem. Heterocycl. Comp.*, **44**, 1275-1283 (2008)].
53. E. B. Averina, O. A. Ivanova, E. M. Budynina, Yu. A. Volkova, T. S. Kuznetsova, and N. S. Zefirov, Acyclic ntronic esters: Generation and utilization in the synthesis of *N*- and *O*-heterocycles, *Vestn. MGU, ser. Khimiya*, **49**, 163-182 (2008).
54. Yu. A. Volkova, O. A. Ivanova, E. B. Averina, E. M. Budynina, T. S. Kuznetsova, and N. S. Zefirov, Study of the Reaction of Trinitromethane with Oxiranes. *Dokl. Chem.*, **419** (2), 83-86 (2008).
55. T. V. Dubinina, R. A. Piskovoi, A. O. Tolbin, V. E. Pushkarev, M. Yu. Vagin, L. G. Tomilova, and N. S. Zefirov, Synthesis of new lanthanide naphthalocyanine complexes based on 6,7-bis(phenoxy)-2,3-naphthalodinitrile and their spectral and electrochemical investigation, *Russ. Chem. Bull., Int. Ed.*, **57**, 1912-1919 (2008).
56. O. N. Zefirova, E. V. Nurieva, V. N. Nuriev, A. A. Ivanov, N. V. Zyk, and N. S. Zefirov, Synthetic approaches to physiologically active polycyclic compounds: VII. Synthesis of 2-(7-hydroxybicyclo-[3.3.1]non-3-ylmethyl)propane-1,3-diols, *Russ. J. Org. Chem.*, **44**, 1134-1138 (2008).
57. N. V. Zyk, A. Yu. Gavrilova, O. A. Mukhina, O. B. Bondarenko, and N. S. Zefirov, A new method for the activation of ethyl benzenesulfenate in electrophilic addition reactions, *Russ. Chem. Bull., Int. Ed.*, **57**, 2572-2578 (2008).
58. E. V. Radchenko, G. V. Makhaeva, V. V. Malygin, V. B. Sokolov, V. A. Palyulin, and N. S. Zefirov, Modeling of the relationships between the structure of O-phosphorylated oximes and their anticholinesterase activity and selectivity using molecular field topology analysis (MFTA), *Dokl. Biochem. Biophys.*, **418** (1), 47-51 (2008).
59. A. V. Ivanov, M. Yu. Tsentalovich, E. G. Kogan, L. G. Tomilova, and N. S. Zefirov, Chlorination of aromatic substrates catalyzed by the phthalocyanine complexes, *Russ. Chem. Bull., Int. Ed.*, **57**, 1676-1679 (2008).
60. A. V. Ivanov, K. V. Kabanova, M. O. Breusova, I. V. Zhukov, L. G. Tomilova, and N. S. Zefirov, New phosphorus-containing metal phthalocyanine complexes. Synthesis and spectral and electrochemical studies, *Russ. Chem. Bull., Int. Ed.*, **57**, 1665-1669 (2008).
61. S. G. Klochkov, V. S. Afanas'eva, and N. S. Zefirov, Study of sesquiterpenoic lactones of plants Indula class as a basis for the creation of novel antineoplastics with proapoptosis activity, *Tekhnologii Zhivykh Sistem*, **5** (5-6), 31-39 (2008).
62. E. P. Kondratovich, I. I. Baskin, N. I. Zhokhova, V. A. Palyulin, and N. S. Zefirov, Application of support vector machine for prediction of the assignment of organic compounds to pharmacological groups, in: *Proc. of the XVII Russian National Congress "Man & Drug". Moscow, Russia, April 14-18* [in Russian], 382 (2008).
63. A. A. Mandrugin, S. Ya. Proskuryakov, T. T. Trofimova, Yu. G. Verkhovskii, N. S. Zefirov, O. N. Zefirova, and V. M. Fedoseev, Antihypotensive drug, Russ. Pat. 02338538 (2008).
64. E. D. Matveeva, T. A. Podrugina, A. S. Pavlova, A. V. Mironov, and N. S. Zefirov, One-pot process for phosphonium-iodonium ylides: nucleophilic substitution and Wittig reaction, *Russ. Chem. Bull., Int. Ed.*, **57**, 400-405 (2008).
65. E. D. Matveeva and N. S. Zefirov, Catalytic Kabachnik-Fields reaction: New horizons for an old reaction, *ARKIVOC*, 1-17 (2008).

66. E. R. Milaeva, O. A. Gerasimova, Z. Jinqwei, D. V. Spakovsky, S. A. Syrbu, A. S. Semeykin, O. I. Koifman, E. G. Kireeva, E. F. Shevtsova, S. O. Bachurin, and N. S. Zefirov, Synthesis and antioxidative activity of metalloporphyrins bearing 2,6-di-*tert*-butylphenol pendants, *J. Inorg. Biochem.*, **102**, 1348-1358 (2008).
67. S. S. Trach and N. S. Zefirov, Symmetry specified enumeration of substituted derivatives: An easy solution to the complex problem, *Russ. Chem. Bull., Int.Ed.*, **57**, (235) (2008).
68. A. N. Fedotov, E. V. Trofimova, K. A. Potekhin, S. S. Mochalov, Yu. S. Shabarov, and N. S. Zefirov, Synthesis of 2-amino-4H-3,1-benzoxazines and 2-amino-4H-3,1-benzothiazines by rearrangement of *o*-cyclopropyl-substituted ureas and thioureas, *Khim. Geterotsikl. Soed.*, 115-126 (2008). [*Chem. Heterocycl. Comp.*, **44**, 96-105 (2008)].
69. D. A. Shulga, A. A. Oliferenko, S. A. Pisarev, V. A. Palyulin, and N. S. Zefirov, Parameterization of empirical schemes of partial atomic charge calculation for reproducing the molecular electrostatic potential, *Dokl. Chem.*, **419** (1), 57-62 (2008).
70. E. V. Radchenko, V. A. Palyulin, and N. S. Zefirov, Molecular field topology analysis in drug design and virtual screening, Chapter 5, *The Royal Soc. Chem. Publishing*, 150-181 (2008).
71. D. Shulga, A. A. Oliferenko, S. A. Pisarev, V. A. Palyulin, and N. S. Zefirov, Fast tool for calculations of atomic charges well suited for drug design, *SAR, and QSAR Environ. Res.*, **19**, 153-165 (2008).
72. Y. A. Volkova, O. A. Ivanova, E. M. Budynina, E. V. Averina, T. S. Kuznetsova, and N. S. Zefirov, A three-component one-pot reaction of trinitromethane, epoxides, and alkenes *via* dinitrinitronates: synthesis of highly functionalized 3,3-dinitroisoxazolidines, *Tetrahedron*, **64**, 3548-3553 (2008).
73. Y. A. Volkova, O. A. Ivanova, E. M. Budynina, E. V. Averina, T. S. Kuznetsova, and N. S. Zefirov, Tetranitromethane as an efficient reagent for the conversion of epoxides into β -hydroxy nitrates, *Tetrahedron Lett.*, **49**, 3935-3938 (2008).
74. A. E. Voronkov, I. I. Baskin, V. A. Palyulin, and N. S. Zefirov, Molecular modelling of modified peptides, potent inhibitors of the xWNT8 and hWNT8 proteins, *J. Mol. Graphics Modell.*, **26**, 1179-1187 (2008).
75. A. E. Voronkov, I. I. Baskin, V. A. Palyulin, and N. S. Zefirov, Molecular modelling of modified peptides, potent inhibitors of the xWNT8 and hWNT8 proteins (Errata), *J. Mol. Graphics Modell.*, **27**, 569 (2008).
76. O. Yakovenko, A. A. Oliferenko, V. G. Bdzhola, V. A. Palyulin, and N. S. Zefirov, Kirchoff atomic charges fitted to multipole moments: Implementation for a virtual screening system, *J. Comput. Chem.*, **29**, 1332-1343 (2008).
77. O. N. Zefirova, E. V. Nurieva, H. Lemcke, A. A. Ivanov, D. V. Shishov, D. G. Weiss, S. A. Kuznetsov, and N. S. Zefirov, Design, synthesis, and bioactivity of putative tubulin ligands with adamantine core, *Biorg. Med. Chem. Lett.*, **18**, 5091-5094 (2008).
78. O. N. Zefirova, E. V. Nurieva, H. Lemcke, A. A. Ivanov, N. V. Zyk, D. G. Weiss, S. A. Kuznetsov, and N. S. Zefirov, Design, synthesis, and bioactivity of simplified taxol analogues on the basis of bicyclo[3.3.1]nonane derivatives, *Mendeleev Commun.*, **18**, 183-185 (2008).
79. E. V. Averina, T. S. Kuznetsova, and N. S. Zefirov, Polynitromethanes – unique reagents in the synthesis of nitro-substituted heterocycles, *Synlett.*, 1543-1557 (2009).
80. E. V. Averina, K. N. Sedenkova, I. S. Borisov, Yu. K. Grishin, T. S. Kuznetsova, and N. S. Zefirov, Unusual methylation reaction of *gem*-bromofluorospiropentanes with methylolithium, *Tetrahedron*, **65**, 5693-5701 (2009).
81. I. I. Baskin, N. I. Zhokhova, V. A. Palyulin, A. N. Zefirov, and N. S. Zefirov, Multilevel approach to the prediction of properties of organic compounds in the framework of the QSAR/QSPR methodology, *Dokl. Chem.*, **427** (1), 172–175 (2009).

82. I. S. Veselov, I. V. Trushkov, and N. S. Zefirov, *trans*-4-Amino-3-hydroxypiperidines. Regio- and stereoselective synthesis, *Russ. J. Org. Chem.*, **45**, 1050-1060 (2009).
83. T. N. Gribanova, N. S. Zefirov, and V. I. Minkin, Quantum-chemical study of heteroanalogs of [8]circulenes and their derivatives, *Dokl. Chem.*, **426** (1), 105-111 (2009).
84. N. I. Zhokhova, I. I. Baskin, D. K. Bakhranov, V. A. Palyulin, and N. S. Zefirov, Method of continuous molecular fields in the search for quantitative structure–activity eelationships. *Dokl. Chem.*, **429** (1), 273-276 (2009).
85. T. Yu. Baranova, N. V. Averina, N. V. Zyk, N. S. Zefirov, K. A. Lyssenko, M. Yu. Antipin, and O. N. Zefirova, Synthesis of indole derivatives fused with the bicyclo[3.3.1]octane framework, *Mendeleev Commun.*, **19**, 10-11 (2009).
86. I. I. Baskin, V. A. Palyulin, and N. S. Zefirov, Molecular modelling of receptors of physiologically active compounds for medicinal chemistry purposes., *Russ. Chem. Rev.*, **78**, 495-511 (2009).
87. E. K. Beloglazkina, A. G. Majouga, A. A. Moiseeva, N. V. Zyk, and N. S. Zefirov, Oxidation of triphenylphosphine and norbornene by nitrous oxide in the presence of Co^{II}Cl₂ [L=3-phenyl-5-(2-pyridylmethyldene)-2-thiohydantoin]: the first example of Co^{II}-catalysed alkene oxidation by N₂O, *Mendeleev Commun.*, **19**, 69-71 (2009).
88. O. B. Bondarenko, A. Yu. Gavrilova, V. V. Polunina, Z. A. Starikova, N. V. Zyk, and N. S. Zefirov, Unexpected mode of reactivity in nitrosation of *cis*-1,1-dichloro-2,3-diphenylcyclopropane with NOCl·2SO₃, *Mendeleev Commun.*, **19**, 12-13 (2009).
89. E. V. Radchenko, G. V. Makhaeva, V. V. Malygin, V. B. Sokolov, V. A. Palyulin, and N. S. Zefirov, Study of the structural determinants of acute and delayed neurotoxicity of O-phosphorylated oximes by molecular field topology analysis (MFTA), *Dokl. Biochem Biophys.*, **429** (1), 309-314 (2009).
90. A. Z. Kadzhaeva, E. V. Trofimova, A. N. Fedotov, K. A. Potekhin, R. A. Gazzaeva, C. C. Mochalov, and N. S. Zefirov Reaction of 2-aryl- cyclopropanecarboxylic acid ethers with HNO₂. Synthesis of aryl-substituted 3-ethoxycarbonyl-4,5-dihydroizoxazoles and 3-ethoxycarbonylisoxazoles, *Khim. Geterotsikl. Soed.*, 753-765 (2009). [*Chem. Heterocycl. Comp.*, **45**, 595-605 (2009)].
91. E. P. Kondratovich, N. I. Zhokhova, I. I. Baskin, V. A. Palyulin, and N. S. Zefirov, Fragmental descriptors in (Q)SAR: prediction of the assignment of organic compounds to pharmacological groups using the support vector machine approach. *Russ. Chem. Bull., Int. Ed.*, **58**, 657-66 (2009).
92. M. I. Lavrov, V. A. Palyulin, V. V. Grigor'ev, S. O. Bachurin, and N. S. Zefirov, Design of new modulators of AMPA receptors that influence the formation of memory, in: *Proc. of the XVI Russian National Congress "Man & Drug". Moscow, Russia, April 6-10* [in Russian], 543-544 (2009).
93. S. S. Mochalov, M. I. Khasanov, and N. S. Zefirov. Synthesis of cyclopropyl-substituted 4H-3,1-benzoxazines from 2-aminophenyl cyclopropyl ketones and 2-cyclopropanoylaminoacylbenzenes, *Khim. Geterotsikl. Soed.*, 252- 268 (2009). [*Chem. Heterocycl. Comp.*, **45**, 201-214 (2009)].
94. D. I. Osolodkin, D. A. Shulga, V. A. Palyulin, and N. S. Zefirov Design of new modulators of AMPA receptors that influence the formation of memory, in: *Proc. of the XVI Russian National Congress "Man & Drug". Moscow, Russia, April 6-10*[in Russian], 543-544 (2009).
95. E. D. Matveeva, T. A. Podrugina, A. S. Pavlova, A. V. Mironov, R. Gleiter, and N. S. Zefirov, Novel photochemical reactions of phosphonium-iodonium ylides: synthesis of phosphonium-substituted oxazoles, *Eur. J. Org. Chem.*, 2323-2327 (2009).
96. E. D. Matveeva, T. A. Podrugina, A. S. Pavlova, A. V. Mironov, A. A. Borisenko, R. Gleiter, and N. S. Zefirov, Heterocycles from phosphonium-iodonium ylides, Photochemical synthesis of λ^5 -phosphinolines, *J. Org. Chem.*, **74**, 9428-9432 (2009).

97. P. V. Oliferenko, A. A. Oliferenko, G. Poda, V. A. Palyulin, N. S. Zefirov, and A. R. Katritzky, New development in hydrogen bonding acidity and basicity of small organic molecules for prediction of physical and ADMET properties, Pt. 2. The universal solvation equation, *J. Chem. Inf. Comput. Sci.*, **49**, 634-646 (2009).
98. D. I. Osolodkin, V. I. Chupakhin, V. A. Palyulin, and N. S. Zefirov, Molecular modelling of ligand-receptor interaction in GABA_C receptors, *J. Mol. Graphics Modell.*, **27**, 813-821 (2009).
99. E. B. Trofimova, V. P. Archegov, A. N. Fedotov, R. A. Gazzaeva, S. S. Mochalov, and N. S. Zefirov, Synthesis of 4H-3,1-benzoxazines from benzylcyclopropanes. The first acid-catalysed rearrangement of *ortho*-substituted benzylcyclopropanes, *Khim. Geterotsikl. Soed.*, 1368-1379 (2009). [*Chem. Heterocycl. Comp.*, **45**, 1095-1104 (2009)].
100. V. Sh. Fel'dblyum, T. N. Antonova, and N. S. Zefirov, Cyclization and dehydrocyclization of C5 hydrocarbons over platinum nanocatalysts and in the presence of hydrogen sulfide. *Dokl. Chem.*, **424** (2), 27-31 (2009.)
101. M. I. Skvortsova, V. A. Palyulin, and N. S. Zefirov, Design of topological indices: computer-oriented approach, *SAR and QSAR Environ. Res.*, **20**, 357-377 (2009).
102. A. Yu. Tolbin, V. E. Pushkarev, L. G. Tomilova, and N. S. Zefirov, Selective synthesis of clam-shell-type phthalocyanines, *Mendeleev Commun.*, **19**, 78-80 (2009).
103. S. S. Tratch, M. S. Molchanova, and N. S. Zefirov, A unified approach to characterization of molecular composition, connectivity, and configuration: Symmetry, chirality, and general problems for the corresponding combinatorial objects, *MATCH*, **61**, 217-266 (2009).
104. F. M. Bickelhaupt, C. F. Guerra, and N. S. Zefirov, C(CN)5: Transition state or intermediate, *Mendeleev Commun.*, **19**, 72-73 (2010).
105. N. I. Zhokhova, I. I. Baskin, A. N. Zefirov, V. A. Palyulin, and N. S. Zefirov, Pseudofragmental descriptors based on combination of atomic properties for prediction of physical properties of polymers in quantitative structure–property relationship studies, *Dokl. Chem.*, **430** (2), 39-42 (2010).
106. A. V. Chemagin, N. V. Yashin, Yu. K. Grishin, T. S. Kuznetsova, and N. S. Zefirov, Diethyl[nitro(diazo)methyl]phosphonate: Synthesis and reactivity toward alkenes, *Synthesis*, 259-266 (2010).
107. N. D. Chuvylkin, E. A. Smolenskii, M. S. Molchanova, and N. S. Zefirov, Geometrical properties of nodal surfaces of many-electron wave functions, *Int. J. Quantum Chem.*, **109**, 1809-1819 (2010).
108. N. V. Zakharevich, D. I. Osolodkin, I. I. Artamonova, V. A. Plyulin, V. N. Danilenko, and N. S. Zefirov, Classification of bacterial eukaryotic type serine/threonine protein kinases – targets for the design of new drugs, in: *Proc. of the XVII Russian National Congress "Man & Drug". Moscow, Russia, April 12-16* [in Russian], 618, (2010)
109. T. V. Dubinina, A. V. Ivanov, N. E. Borisova, S. A. Trashin, S. I. Gurskiy, L. G. Tomilova, and N. S. Zefirov, Synthesis and investigation of spectral and electrochemical properties of alkyl-substituted planar binuclear phthalocyanine complexes sharing a common naphthalene ring, *Inorg. Chim. Acta*, **363**, 69-71 (2010).
110. T. N. Gribanova, N. S. Zefirov, and V. I. Minkin, Structure and stability of heteroannulated [8-10]ciculenes: a quantum-chemical study, *Pure Appl. Chem.*, **82**, 1011-1024 (2010).
111. E. D. Matveeva, R. Gleiter, and N. S. Zefirov A novel photochemical reaction of a mixed phosphonium iodonium ylide with phenylacetylene as a route to diphenyl-1 λ^5 -phosphinoline. *Russ. Chem. Bull., Int. Ed.*, **59**, 488 (2010).
112. E. D. Matveeva, T. A. Podrugina, I. N. Kolesnikova, and N. S. Zefirova, Hydrophosphorylation of hydrazones and azines, catalyzed by phthalocyanines, *Izv. Akad. Nauk, Ser. Khim.*, 571-576 (2010).
113. E. D. Matveeva, T. A. Podrugina, I. N. Kolesnikova, and N. S. Zefirov, Benzoylhydrazones in catalytic hydrophosphorylation *Russ. Chem. Bull., Int. Ed.*, **59**, 411-417. (2010).

114. E. D. Matveeva, T. A. Podrugina, M. V. Prisyazhnoi, S. O. Bachurin, and N. S. Zefirov, Synthesis of a "memory tripeptide" (Arg-Glu-Arg, RER) and the Kabachnik-Fields reaction with di- and tripeptides as a method for the synthesis of phosphorus-containing peptide analogs. *Russ. Chem. Bull., Int. Ed.*, **59**, 200-208 (2010).
115. E. D. Matveeva, T. A. Podrugina, I. N. Kolesnikova, M. V. Prisyazhnoi, G. G. Karateev, and N. S. Zefirov, Catalytic hydrophosphorylation of alkyl- and acylhydrazones. *Russ. Chem. Bull., Int. Ed.*, **59**, 418-424 (2010).
116. D. A. Tsareva, D. I. Osolodkin, D. A. Shulga, A. A. Oliferenko, V. A. Palyulin, and N. S. Zefirov, The role of partial atomic charges in the 3D QSAR modelling, in: *Proceedings of the XVII Russian National Congress "Man & Drug", Moscow, Russia, April 12-16*, 740 (2010).
117. A. Yu. Tolbin, V. E. Pushkarev, L. G. Tomilova, and N. S. Zefirov, New approach to the synthesis of planar binuclear phthalocyanines of Mg, Zn, and rare-earth elements, *Macroheterocycles*, **3**, 30-32 (2010).
118. Y. A. Volkova, E. B. Averina, T. S. Kuznetsova, and N. S. Zefirov, Ring opening of aziridines with tetranitromethane in the presence of triethylamine, Efficient synthesis of β -tosylaminonitrates, *Tetrahedron Lett.*, **51**, 2254-2257 (2010).