C U R R I C U L U M V I T A E

1. PERSONAL DATA

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2. EDUCATION AND POSITIONS HELD:

1968 - 1973: Student at Odessa University, Departments of Chemistry
1973 - 1976: Postgraduate Student of the Dept. Organic Chemistry, Odessa Univ.
1976 - 1978: Researcher, Dept. of Organic Chemistry, Odessa Univ.
1978 - 1988: Researcher, A.V.Bogatsky Physico-Chemical Institute Academy of Sciences of Ukraine
1988 - 1996: Head of Laboratory on Theoretical Chemistry, Phys.-Chem. Inst.
1996 - 2001: Head Scientist, Deputy Head of Department on Thermodynamics and Theoretical Chemistry,
2001 - 2007: Head Scientist, Deputy Head of Department on Molecular Structure, Head of Laboratory on Theoretical Chemistry
2007 – 2012: Vice Director on Research, Head of Laboratory on Theoretical Chemistry
2012 – Present: Head of Department on Molecular Structure and Chemoinformatics

As by-worker:

1997 - 2008: Assistant Professor, Department on Organic Chemistry, I. I. Mechnikov Odessa National University
2008 – present: Full Professor, Department on Organic Chemistry, I. I. Mechnikov Odessa National University

3. PROFESSIONAL DEGREES:

1980. Degree of Candidate of Sciences (Ph.D) in Organic Chemistry. Thesis "Conformational Peculiarity of Seven Membered and Stereochemistry of Six Membered of 4- trifluormethyl-1,3-dioxacyclanes".
1986. Senior Researcher.
2004. Degree of Doctor of Chemical Science in Organic Chemistry. Thesis "Topological and conformation aspects of macrocycles functioning".
2007. – Professor in Bioorganic Chemistry

4. SCIENTIFIC INTERESTS:

Molecular topology, Molecular mechanics, Mathematical chemistry, Chemometrics, Theoretical stereochemistry and conformational analysis, Supramolecular chemistry, Theory of information, QSAR/QSPR and Drug Design problems.

5. THE BASE DIRECTION OF SCIENTIFIC ACTIVITY.

Main area of activity:

Development and realization of approaches, methods and computer programs for:

- Analysis and modeling of molecular structure;
- Solution of "structure – activity/property" (QSAR/QSPR) tasks;
- Molecular design of compounds (potential reagents, materials, preparations) with the given complex of properties.

Main original developments:

- **Conception of the informational field of molecule** is based on the probabilistic-statistical Shannon information

theory. Actually, within the framework of this conception using formal positions a situation is described, when an object (molecule) structurize surrounding space, i.e. generates the potential information due to the complex of the real physical fields. However, approach is not explore how the structurizing of surrounding space is occurring, but analyze only its consequences. On the basis of different characteristics of the molecular informational fields possibility of generation of large array of new structural parameters that are very effective for different QSAR/QSPR studies is realized.

- **Hierarchical system of the QSAR/QSPR models (1D - 4D).** The essence of this system is that the QSAR problem is solved sequentially in a series of improved models of the description of molecular structure. Thus, on each subsequent stage of a hierarchic system the QSAR problem is solved not *ab ovo*, but the information obtained on the previous step has been used. Actually, we deal with a system of solutions that defined more exactly. The proposed approach allows more effectively interpretation of obtained QSAR models, because it becomes more evident, for what molecular fragments the detailed elaboration of structure is important. Besides, the comparing of results of subsequent QSAR solutions allows to decide is it expedient to complicate molecular models for increasing an adequacy of QSAR.
- **Simplex approach for modeling of molecular structure.** A molecule is represented as the system of different simplexes - tetratomic fragments of fixed structure, chirality and symmetry. Such approach allows unifying the description of spatial structure of compounds with saving of the complete stereochemical information that allows to develop different descriptors of molecular structure for the effective decision of QSAR/QSPR tasks. It enables to determine easily common fragments of structure both promoting and interfering to given property (for example, activity) for molecules. Realizing of molecular design of compounds with the given level of activity using the generation of the allowed combinations of simplexes that determines investigated property, is possible on the base of this method. The developed approach has not the limitations (ambiguous of optimal alignment of the set of considered molecules) of one of the most popular methods of QSAR researches – *CoMFA*. The approach is similar to HQSAR (holographic QSAR) but has no it restrictions (only topological representation of molecular structure) and lacks (ambiguity of descriptors formation when procedure of hashing of molecular holograms is realized).
- **System of stereoanalyse and stereodesign of chiral molecules.** Universal approach for quantitative **estimation** of molecular structure asymmetry relatively to different elements of point groups of symmetry is developed. Within the framework of this approach the chirality of molecule is estimated quantitatively. This parameters is used for the QSAR/QSPR studies in which the explored properties are determined by chirality of molecule.
  Symbiosis of simplex presentation of molecular structure with possibility of quantitative estimation of chirality allows uniquely determine stereochemical configuration of molecules and their fragments of any degree of complexity (stereoanalyse), and also construct new molecular structures with the defined level of chirality (stereodesign).
- **Universal approaches to description of form of molecules and their structural similarity/dissimilarity with each other.** The harmonic analysis (Fourier transform) of discrete function of conformational parameters of molecules of different structural classes allows from single positions to describe and compare characteristics of their form, such as aplanarity, sphericity, bulge/concavity, folding, etc. Different metrics constructed on amplitudes of the Fourier transform harmonics and/or on the basis of autocorrelation functions allow to estimate structural similarity/dissimilarity for the pair of molecules of arbitrary structure. It enables effectively to decide the QSAR/QSPR tasks on the basis of principle of structural similarity since the compounds that are similar from the standpoint of defined structural descriptions are close by the corresponding properties.

All developed approaches and models (greater part of its does not have analogues) are realized as the computer programs for the personal computers IBM PC in the Windows XP, 2000, 7 environment.
Thus, the created "toolkit" allows to decide the most various "structure-properties" tasks.
<u>The solved tasks:</u>

- The structural aspects of functioning of macrocyclic polyesters (including, crown-ethers) and their analogues, as complexones, isotope-differentiating and enantio-differentiating agents, catalysts of phase-transfer, antimicrobial agents, etc.
- Analysis of structure influencing on ability of molecules to formation of different types of mesophases: nematic, smectic, «banana», and also temperatures of interphase transitions. Constructing of chiral molecules that able effectively «twist» of nematic mesophase.
- Sterochemical analysis of fullerenes with chiral skeleton. Reveal of structural factors that determining the level of chirality of these compounds
- The analysis of relation "structure-smell" for different synthetic odorants.
- Investigations of thermodynamic properties of hydrocarbons, halogenhydrocarbons and chladones.
- Prognosis of luminescence properties in the series of complexes of ions of rare earth elements with β-diketonates and macroheterocycles.
- QSAR researches: macrocyclic pyridinophanes (anticancer and antivirus activity); synthetic nucleosides (antivirus activity); 1,4 - benzdiazepines (psychotropic activity and affinity to the $GABA_A$ receptors); some aromatic

heterocycles (interferon induction); thiazolidone derivatives (antiphlogistic activity); substituted piperazines (affinity to serotonins 5-HT_{1A} receptors); amynoalkylindoles (affinity to the cannabinoids CB_1 receptors) and others.

Some of the main pulications:

1. Alikhanidi S., Kuz'min V. An Optimization of Asymmetry Evaluation of Molecules within the Folding-Unfolding Method // J. Mol. Mod.- 1999.-№5.-P.116-124.
2. Vityuk N., Voskresenskaja E., Kuz'min V. The Synergism of Methods Barycentric Coordinates and Trend-vector for Solution "Structure-Property" Tasks //Pattern Recognition and Image Analysis.- 1999.-9, №3.-P.521-528.
3. V.E. Kuz'min, A.G. Artemenko, N.A. Kovdienko, I.V. Tetko, D.J. Livingstone. Lattice Model for QSAR Studies.// J. Mol. Model., 2000, № 6, p. 517-526.
4. V.E. Kuz'min, V.P.Lozitsky, G.L.Kamalov, R.N.Lozitskaya, A.I.Zheltvay, A.S.Fedtchouk, D.N.Kryzhanovsky. The analysis of "structure - anticancer activity" relationship in a set of macrocyclic 2,6-bis (2- and 4-formylaryloxymethyl) pyridines schiff bases.// Acta Biochimica Polonica, 2000, 47, №3, p.867-875.
5. Alikhanidi S, Kuz'min V. Stereodesign of chiral para-substituted calyx[4]arenas. J. Mol. Modeling.- 2001, - v.7, №5.- P.143-146.
6. Kuz'min V.E., Ognichenko L.N., Artemenko A.G. Modeling of the informational field of molecules. J. of Molecular Modeling.- 2001.- v.7, №7.- P.278-285
7. Kuz'min V.E, Artemenko A.A., Lozitsky V.P., Muratov E.N., Fedtchouk A.S., Dyachenko N.S., Nosach L.N., Gridina T.L., Shitikova L.I., Mudrik L.M., Chelombitko V.A., Zheltvay A.I., Vanden Eynde J.J. The analysis of structureanticancer and antiviral activity relationships for macrocyclic pyridinophanes and their analogues on the basis of 4D QSAR models (simplex represemtation of molecular structure). Acta Biochimica Polonica. -2002. -49, №1. -P. 157-168.
8. Kuz'min V.E., Artemenko A.G., Lozitska R.N., Fedtchouk A.S., Lozitsky V.P., Muratov E.N., Mescheriakov A.K. Investigation of Anticancer Activity by Means of 4D QSAR Based on Simplex Representation of Molecular Structure //SAR and QSAR in Env. Res.-2005- Vol. 16, No 3.-P. 219-230.
9. Artemenko A.G., Muratov E.N., Kuz'min V.E., Kovdienko N.A., Hromov A.I., Makarov V.A., Riabova O.B., Wutzler P., Schmidtke M. Identification of individual structural fragments of N,N'-(bis-5-nitropyrimidyl)dispirotripiperazine derivatives for cytotoxicity and antiherpetic activity allows the prediction of new highly active compounds. // J. Antimicrob. Chemother.- 2007.- V. 60, №1.- P. 68-77
10. Kuz'min V., Artemenko A., Muratov E., Volineckaya I., Makarov V.A., Riabova O.B., Wutzler P., Schmidtke M. Quantitative Structure-Activity Relationship Studies of [(Biphenyloxy)propyl]isoxazole Derivatives. Inhibitors of Human Rhinovirus 2 Replication. // J. Med. Chem. -2007.- V.50.- P. 4205 – 4213.
11. Kuz'min V.E., Artemenko A.G, Muratov E.N. Hierarchical QSAR tech-nology based on the Simplex representation of molecular structure. // J. Comput. Aided Mol. Design.- 2008.-V.22.- P. 403-421.
12. Polischuk P. G., Artemenko A. G., Makan S.Yu., Kuz'min V.E., Andronati S.A. Quantitative structure-affinity relationship of 5-HT1A receptor ligands by the classification tree method. // SAR and QSAR in Environmental Research.-2008.- Vol. 19, № 3–4, April–June.- P. 213–244
13. Kuz'min V.E., Muratov E.N., Artemenko A.G., Gorb L., Qasim M., Leszczynski J. The effect of nitroaromatics' composition on their toxicity in vivo: Novel efficient non-additive 1D QSAR analysis.// Chemosphere .- 2008.- Vol. 72.- P.1373–1380.
14. Anatoliy G. Artemenko, Eugene N. Muratov, Dmytro V. Atamanyuk, Victor E. Kuz_min, Alexander I. Hromov, Roman V. Kutsyk and Roman B. Lesyk. QSAR Analysis of Antimicrobial Activity of 4-thiazolidone Derivatives. //QSAR Comb. Sci. -2009.- Vol. 28, No. 2.- P.194 – 205.
15. Kholod Y.A., Muratov E.N., Gorb L.G., Hill F.C., Artemenko A.G., Kuz'min V.E., Qasim M., Leszczynski J.Application of Quantum Chemical Approximations to Environmental Problems: Prediction of Water Solubility for Nitro Compounds. //Environ. Sci. Technol. – 2009. – DOI: 10.1021/es902566b
16. Kuz'min V.E., Muratov E.N., Artemenko A.G., Varlamova E.V., Gorb L., Wang J., Leszczynski J. Consensus QSAR Modeling of Phosphor-Containing Chiral AChE Inhibitors.//QSAR Comb. Sci. 2009. - Vol. 28, P. DOI: 10.1002/qsar.200860117.
17. Polishchuk P.G., Muratov E.N., Artemenko A.G., Kolumbin O.G., Muratov N.N., Kuz'min V.E. Application of Random Forest Approach to QSAR Prediction of Aquatic Toxicity.//J. Chem. Inf. Model. – 2009. – Vol. 49. – P. 2481 - 2488.
18. Artemenko A.G., Muratov E.N., Polischuk P.G. Kuz'min V.E. et al, Virtual screening and molecular design based on hierarchical QSAR technology, «Recent Advances in QSAR Studies», Springer, London, 2010, pp. 127-176.
19. Muratov E., Varlamova E., Kuz'min V., Artemenko A., Nikolaeva-Glomb L., Galabov A. QSAR Analysis of Poliovirus Inhibition by Dual Combinations of Antvirals. //Antiviral Research. - 2010. - Vol. 86. - P. A62.
20. Muratov E.N., Artemenko A.G., Varlamova E.V. Kuzmin V.E. et al, Per aspera ad astra: application of Simplex QSAR approach in antiviral research.// Future Medicinal Chemistry. - 2010. - Vol. 2. - P. 1205 – 1226.

21. Polishchuk P.G., Artemenko A.G. Andronati S.A. Kuz'min V.E. Interpretation of QSAR models based on Random Forest method. //Molecular Informatics. - 2011. - Vol. 30. - P. 593 – 603.
22. Muratov E.N., Kuz'min V.E. Varlamova E.V., Khristova T. et al, QSAR analysis of [(biphenyloxy)propyl]isoxazoles: agents against coxakievirus B3.// Future Med. Chem. - 2011. - V. 3, №1.- P. 31 - 43.
23. Ognichenko L.N., Kuz'min V.E., Gorb L., Muratov E.N., Artemenko A.G., Kovdienko N.A., Polishchuk P.G., Hill F.C., Leszczynski J. New advances in QSPR/QSAR analysis of nitrocompounds: solubility, lipophilicity and Toxicity. In Practical aspects of computational chemistry II, Eds. J. Leszczynski, M. Shukla, Springer, London, 2012, P. 279-334.
24. Gorb L.,. Hill F.C., Holod Y., Muratov E.N., Kuz'min V.E., Leszczynski J. Progress in Prediction of Environmentally Important Phisicochemical Properties of Energetic Materials: Applications of Quantum-Chemical Calculations. In Practical aspects of computational chemistry II, Eds. J. Leszczynski, M. Shukla, Springer, London, 2012, P. 335-360.
25. Muratov E.N., Varlamova E.V., Artemenko A.G., Polishchuk P.G., Kuz'min V.E. Existing and Developing Approaches for QSAR Analysis of Mixtures. Molecular Informatics. – 2012.- V. 31, P. 202 – 221.
26. Ognichenko L.N., Kuz'min V.E., Gorb L., Hill F.C., Artemenko A.G., Polischuk P.G. and Leszczynski J. QSPR Prediction of Lipophilicity for Organic Compounds Using Random Forest Technique on the Basis of Simplex Representation of Molecular Structure. Molecular Informatics. - 2012. - Vol. 31. - P. 273 - 280.
27. Oprisiu I., Varlamova E., Muratov E., Artemenko A., Marcou G., Polishchuk P., Kuz'min V. and Varnek A. QSPR Approach to Predict Nonadditive Properties of Mixtures. Application to Bubble Point Temperatures of Binary Mixtures of Liquids. Molecular Informatics. — 2012. — Vol.31. — P. 491 – 502.
28. Muratov E. N. Varlamova E. V. Artemenko A. G. Polishchuk P. G. Nikolaeva-Glomb L. Galabov A. S. Kuz'min V. E. QSAR analysis of poliovirus inhibition by dual combinations of antivirals.Structural Chemistry.- 2013.-V.53. - P.1665-1679.
29. Polishchuk P.G., Kuz'min V.E., Artemenko A.G., Muratov E.N. Universal Approach for Structural Interpretation of QSAR/QSPR Models. Molecular Informatics. - 2013. – V.32, № 9-10. – P. 843-853.
30. Cherkasov Artem, Muratov Eugene N., Fourches Denis, Varnek Alexandre, Baskin Igor I., Cronin Mark, Dearden John, Gramatica Paola, Martin Yvonne C., Todeschini Roberto, Consonni Viviana, Kuz'min Victor E., Cramer Richard, Benigni Romualdo, Yang Chihae, Rathman James, Terfloth Lothar, Gasteiger Johann, Richard Ann and Tropsha Alexander QSAR Modeling: Where Have You Been? Where Are You Going To? J. Med. Chemistry.- 2014.- V.57.-P.4977-5010

Number of research papers in refereed journals: **283**
Number of communications to scientific meetings: **417**
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6. INTERNATIONAL GRANTS.

- International Scientific Foundation (George Soros) (1993). Short-term personal grant.
- International Sciences Foundation Grant U 1O 200 (1994-1995). "New Concepts of Stereochemical Configurations. Stereoanalysis and Stereodesign of Chiral Molecules".
- International Association for the Promotion of Co-operation with Scientists from the Newly Independent States of the former Soviet Union (INTAS Foundation) Grant INTAS-UA 95-0060 (1995-1998). "Development and Application of a Volume-Learning Algorithm for Artificial Neural Networks in 3D Quantitative Structure-Activity Relationship Studies".
- INTAS Foundation, Grant INTAS-UA 97-1730 (1997-2000). "New derivatives of *p*-menthan-3-ones as chiral components of liquid crystalline systems".
- INTAS Foundation Grant INTAS-UA 97-31528 (1997-2000). "Anticancer and Antiviral Properties of Macrocyclic Pyridinophanes. Structure-Activity Relationships and Drug Design".
- International Sciences Foundation Grant QSU083102 (1998). Individual grant for scientist and teachers.
- Grant of Science and Technology Center in Ukraine (STCU). Project # 3147 (2004-2006): "Elaboration of a System for Drug-Design and Selection of Effective Antiherpetic Preparations Using Modern Computer Technologies"

- Grant of Science and Technology Center in Ukraine (STCU). Project P500 (2011-2013): "Distributions, concentrations and health effects of emerging and conventional contaminants in the riverine and estuarine surface waters and fishes of Ukraine"
- Grant of Science and Technology Center in Ukraine (STCU). Project P407 (2012-2014): "Purposeful Search and Structural Drug Design of New Anti-Influenza Agents Based on QSAR Hierarchic System Using Modern Computer Technologies"
- Grant FP7 , Marie Curie International Research Staff Exchange Scheme (2011 – 2014)"Building bridges between specialists in computational and empirical risk assessment of engineered nanomaterials"

7. SCIENTIFIC SCHOOL:

Lyudmila P. Trigub Ph.D 1986
Gennadij M. Verkhivker Ph.D 1986
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Tatiana M. Khristova PhD (France) 2013
Ekaterina V. Varlamova PhD 2014
Irina Yu. Borisiuk Doctor of Pharm. Sci. 2014