# CURRICULUM VITAE

| | |
|---|---|
| ***Surname, firstname, patronymic*** | **Dr. Toropova Alla P. (Toropova Alla Petrovna)** |
| ***Brief service record*** | 1986 - 1991 – Lecturer in Industry College, Uzbekistan<br>1991 - 1994 – PhD student in Tashkent State University, Uzbekistan<br>1994 – 1998 – scientific collaborator at Institute of Geology & geophysics of Acad. Sci. Rep. Uzbekistan<br>1998 - 2007 senior scientific researcher at Institute of Geology & geophysics of Acad. Sci. Rep. Uzbekistan<br>2007–up to present, invited scientist at Istituto di Ricerche Farmacologiche Mario Negri *IRCCS*, Milano, Italy |
| ***Scientific interest*** | Quantitative Structure –Property/Activity Relationships (QSPR/QSAR), modeling of endpoints such as toxicity, mutagenicity, HIV-1 as well as physicochemical properties, inorganic and organometallic compounds; QSPR/QSAR analysis of nano materials.<br>Web design: http://www.insilico.eu/CORAL |
| ***Scientific degree*** | **Ph.D. in chemistry** (1998) |
| ***Membership in Editorial Board of scientific journals*** | 2021, **Guest Editor** of an issue of Frontiers in Bioscience-Landmark (impact factor = 4.009); Special issue: "Drug-induced Diseases: Computational Approaches for Averting It".<br>https://www.imrpress.com/journal/FBL/special_issues/1396741473864962049<br>2021, **Guest Editor** of an issue of Molecules (impact factor =4.412); Special issue: "QSAR and QSPR: Recent Developments and Applications II"; this special issue belongs to the section "Computational and Theoretical Chemistry".<br>https://www.mdpi.com/journal/molecules/special_issues/QSAR_QSPR_II<br>2021, **Guest Editor** of an issue of Chemistry; Special issue: "QSAR and QSPR: Recent Developments and Applications 2021 "; this special issue belongs to the section "Theoretical Chemistry".<br>https://www.mdpi.com/journal/chemistry/special_issues/QSAR_QSPR_Applications<br>2020, **Guest Editor** of an issue of Mini-Reviews in Medicinal Chemistry (MRMC) (impact factor =3.86); Special issue: “Medicinal Chemistry and Computational Chemistry: Mutual Influence and Harmonization”; Vol. 20, No. 14.<br>2018, **Guest Editor** of an issue of International Journal of Quantitative Structure-Property Relationships; Special issue: “Applications of QSPR/QSAR in Toxicology, Ecology, and Drug Discovery: Problems and Solutions”; Volume 3, Issue 2.<br>2017, **Guest Editor** of an issue of Current Drug Metabolism (impact factor =3.731); Special issue: “Impact of Drug Metabolism and its Relevance upon Drug Discovery”; Vol. 18, No. 12<br>2015, **Guest Editor** of an issue of Current Topics in Medicinal Chemistry (CTMC) (impact factor =3,295); Special issue: “From Chemoinformatics to Nanoinformatics: New tools for Drug Discovery and Nanoparticles Design in Medicinal Chemistry”; Vol. 15, No. 18.<br>***Member of the Advisory Editorial Board*** of the journal " Current Protein & Peptide Science" http://www.eurekaselect.com/node/619/current-protein-peptide-science/editorial-board<br>***Member of Editorial Review Board*** of the Journal of Nanotoxicology and Nanomedicine(JNN) http://www.igi-global.com/journal/journal-nanotoxicology-nanomedicine-jnn/126553<br>***Member of the Editorial Board*** of the journal " Molecules" https://www.mdpi.com/journal/molecules/editors<br>***Referee in***<br>Nanoscale |

Chemosphere
RSC Advances
Computers in Biology and Medicine
Medicinal Chemistry Research
Combinatorial Chemistry & High Throughput Screening
Journal of Chemical Information and Modeling
Current Topics in Medicinal Chemistry
Drug Research
Chemometrics and Intelligent Laboratory Systems
Chemical Biology and Drug Design
International Journal of Quantitative Structure-Property Relationships (IJQSPR)
Bioorganic and Medicinal Chemistry

***Address*** 20156, Via Mario Negri, 2, Milan, Italy

***Emails*** **alla.toropova@marionegri.it**
**allatoropova@ymail.com**

## Participation in conferences and workshops

April 11, 2023-MRS Spring Meeting & Exhibit in San Francisco.
https://www.mrs.org/meetings-events/spring-meetings-exhibits/2023-mrs-spring-meeting/call-for-papers/presentations/detail/2023_mrs_spring_meeting/3838685-202304110845
September 21 – 23, 2022, 28th Annual Meeting of the Slovenian Chemical Society, Portorose, Slovenia.
November 11-12, 2021, Nanosafety workshop - From Molecules to Public Health. Portugal, Braga.
26-30 May 2019, The SETAC Europe 29th Annual Meeting, Helsinki, Finland.
June 24, 2016, XLI ELBA Nanoforum on Emerging Lines of Collaborative Russians/Italians Research, Pradalunga (Bergamo), Italy
5–15 December 2015. MOL2NET, International Conference on Multidisciplinary Sciences, C: Polymers, Materials, and Nanosciences. http://sciforum.net/conference/MOL2NET-1/MOL2NET-c
November 4-6, 2015, CompNanoTox-2015, Malaga, Spain
7 - 11 July 2015, 12$^{th}$ International Conference on Nanosciences (NN15). Thessaloniki, Greece
April 29, 2015, CALEIDOS (Final Workshop- 2015), Milan , Italy
June 16-20, 2014, QSAR 2014 , Milan, Italy
June 4-6, 2013, Harmonisation meeting with representatives of other projects in the NMP.2012.1.3-2 Programme "Modelling toxicity behaviour of engineered nanoparticles": ModEnpTox, Modern, NanoPuzzles, PreNanoTox in Brussels, Belgium.
May, 2011, SETAC , Milan, Italy
March, 2011, Orchestra, Milan, Italy
September, 2009, VII World Congress on Alternatives & Animal Use in the Life Sciences, Rome, Italy (poster)
May, 2009, SETAC, Goteborg, Sweden
March, 2008, SCARLET – Istituto di Ricerche Farmacologiche Mario Negri, Milan, Italy

## Participation in International scientific grants

CAESAR (EC Project no. 022674 - SSPI)
OSIRIS (n. 037017 -GOCE)
ANTARES (Grant Agreement LIFE08 ENV/IT/00435)
PROSIL (projectLIFE12ENV/IT/000154)
Federchimica-AISPEC
NanoBRIDGE ( Grant Agreement : PIRSES-GA-2011-295128)
NanoPUZZLES(EC Project Reference:309837)
PreNanoTox (EC Project Reference: 309666)
CALEIDOS (Grant Agreement LIFE 11 ENV/IT/000295)
EC project PeptiCAPS (Project Reference: H2020-686141)
LIFE-COMBASE (LIFE15 ENV/ES/000416)
EC project EU-ToxRisk- H2020-681002
EFSA contract (NP//EFSA/AFSCO/2016/1)
LIFE-VERMEER contract (LIFE16 ENV/IT/000167)

**Characterization of Dr. Toropova A.P. by Google Scholar Citations**
https://scholar.google.com/citations?user=0W8tjIAAAAAJ&hl=it

| Citation indices | All | Since 2019 |
|---|---|---|
| Citations | 7072 | 3845 |
| h-index | 43 | 31 |
| i10-index | 205 | 132 |

**Characterization of Dr. Toropova A.P. by SCOPUS database**
http://www.scopus.com/authid/detail.url?authorId=6701335146
h-Index =39 (i.e. there are 39 articles which are cited 39 or more times)

| Year | The number of published articles and chapters | The total number of citations up to now |
|---|---|---|
| 2024 | 1+3 (in press) | 175 |
| 2023 | 34 | 776 |
| 2022 | 19 | 545 |
| 2021 | 20 | 604 |
| 2020 | 28 | 696 |

**The total number of citations (SCOPUS) is 5939** (April 16, 2024)

## PUBLICATION LIST OF ALLA P. TOROPOVA
## Chapters in Books and other publications:

- **In Book**: *Toropova, A.P., Toropov, A.A. (eds).* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol. 33, pp.1-467. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4

- Toropov, A.A., Raskova, M., Raska, I., Toropova, A.P.
***Chapter 1***. Fundamentals of Mathematical Modeling of Chemicals Through QSPR/QSAR. **In:** *Toropova, A.P., Toropov, A.A.* (*eds*) QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol. 33, Pages 3–24. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_1

- Toropov, A.A., Toropova, A.P.
***Chapter 3***. Application of SMILES to Cheminformatics and Generation of Optimum SMILES Descriptors Using CORAL Software. **In:** *Toropova, A.P., Toropov, A.A. (eds)* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol 33, Pages 57-82. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_3

- Kudyshkin, V.O., Toropova, A.P.
***Chapter 7***. Building Up QSPR for Polymers Endpoints by Using SMILES-Based Optimal Descriptors. **In:** *Toropova, A.P., Toropov, A.A. (eds)* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol 33, Pages 167-187. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_7

- Behera, S.A., Toropova, A.P., Toropov, A.A., Achary, P.G.R.

***Chapter 9.*** Quasi-SMILES-Based Mathematical Model for the Prediction of Percolation Threshold for Conductive Polymer Composites. **In:** *Toropova, A.P., Toropov, A.A. (eds)* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol 33, Pages 211-239. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_9

- Achary, P., Krishna, P., Toropova, A.P., Toropov, A.A.

***Chapter 10.*** On the Possibility to Build up the QSAR Model of Different Kinds of Inhibitory Activity for a Large List of Human Intestinal Transporter Using Quasi-SMILES. **In:** *Toropova, A.P., Toropov, A.A. (eds)* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol 33, Pages 241-268. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_10

- Toropova, A.P., Toropov, A.A.

***Chapter 14***. The CORAL Software as a Tool to Develop Models for Nanomaterials' Endpoints. **In:** *Toropova, A.P., Toropov, A.A. (eds)* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol 33, Pages 351-371. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_14

- Toropov, A.A., Toropova, A.P., Leszczynska, D., Leszczynski, J.

***Chapter 16.*** On Complementary Approaches of Assessing the Predictive Potential of QSPR/QSAR Models. **In:** *Toropova, A.P., Toropov, A.A. (eds)* QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, **2023**, vol 33, Pages 397-420. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_16

- Nilima R. Das, Tripti Sharma, Ayeshkant Mallick, Alla P. Toropova, Andrey A. Toropov, and P. Ganga Raju Achary,

***Chapter 32***. Computational Approach in Designing and Development of Novel Inhibitors of AKR1C1. **In Book**: Tripti Swarnkar, Srikanta Patnaik, Indian Institute of Technology (IIT), *Sanjay Misra, Siksha O. (Eds)*, Ambient Intelligence in Health Care: Proceedings of ICAIHC 2022: 325-339. (Smart Innovation, Systems and Technologies, vol. 317). Springer; 1st ed. **2023** edition. https://doi.org/10.1007/978-981-19-6068-0

- Alla P. Toropova and Andrey A. Toropov,

***Chapter 3.*** Use of the Monte Carlo Method to Build up QSPR/QSAR Models: Index of Ideality of Correlation and Correlation Intensity Index. **In Book**: *Thomas B. Hall (Ed.)*, Monte Carlo Methods: History and Applications. Series: Mathematics Research Developments. Nova, **2020**, pp.111-156. ISBN: 978-1-53617-723-7 https://novapublishers.com/shop/monte-carlo-methods-history-and-applications/

- Andrey A. Toropov, Alla P. Toropova, Alessandra Roncaglioni, and Emilio Benfenati,

***Chapter 27***. Prediction of Biochemical Endpoints by the CORAL Software: Prejudices, Paradoxes, and Results. **In Book**: *Orazio Nicolotti (ed.)*, Computational Toxicology: Methods and Protocols, Methods in Molecular Biology, **2018**, vol. 1800, pp. 573-583. https://doi.org/10.1007/978-1-4939-7899-1_27, © Springer Science+Business Media, LLC, part of Springer Nature

- Andrey A. Toropov and Alla P. Toropova,

***Chapter 8.*** Improved Model for Biodegradability of Organic Compounds: The Correlation Contributions of Rings. **In Book**: *Bidoia E., Montagnolli R. (Eds)* Toxicity and Biodegradation Testing. Methods in Pharmacology and Toxicology. Humana Press, New York, NY. **2018**, pp. 147-183. DOI: 10.1007/978-1-4939-7425-2_8

- Alla P. Toropova, Andrey A. Toropov, Emilio Benfenati, Robert Rallo, Danuta Leszczynska and Jerzy Leszczynski,
***Chapter* 12**. Development of Monte Carlo Approaches in Support of Environmental Research. **In Book**: *Roy, K.* (*eds*) Advances in QSAR modeling. Advances in Computational Chemistry and Physics. Springer International Publishing AG, **2017,** Volume 24, pages 453-469.

- Alla P. Toropova, Andrey A. Toropov, Aleksandar M. Veselinović, Jovana B. Veselinović, Danuta Leszczynska, Jerzy Leszczynski,
***Chapter 8.*** Quasi-Smiles as a novel tool for Prediction of Nanomaterials' endpoints. **In Book**: *Speck-Planche A.* (*eds*) Multi-Scale Approaches in Drug Discovery: From Synthetic Methodologies and Biological Assays to In Silico Experiments and Back. Elsevier Science & Technology Books, **2017,** pages 191-221. ISBN: 0081011296, 9780081011294

- Alla P. Toropova, P. Ganga Raju Achary, Andrey A. Toropov,
***Chapter 59.*** Quasi-SMILES for Nano-QSAR Prediction of Toxic Effect of $Al_2O_3$ Nanoparticles. **In Book:** Pharmaceutical Sciences: Breakthroughs in Research and Practice (2 Volumes) **2017**, pages 1573-1584. DOI: 10.4018/978-1-5225-1762-7

- A.A. Toropov, A.P. Toropova, E. Benfenati, O. Nicolotti, A. Carotti, K. Nesmerak, A.M. Veselinović, J.B. Veselinović, P.R. Duchowicz, D. Bacelo, E.A. Castro, B.F. Rasulev, D. Leszczynska, J. Leszczynski,
***Chapter 36.*** QSPR/QSAR Analyses by Means of the CORAL Software: Results, Challenges, Perspectives. **In Book**: Pharmaceutical Sciences: Breakthroughs in Research and Practice (2 Volumes) **2017,** pages 929-955. DOI: 10.4018/978-1-5225-1762-7

- Toropov A.A., Toropova A.P., Nesmerak K., Veselinović A.M., Veselinović J.B., Leszczynska D., Leszczynski J.,
***Chapter 12***. Development of the latest tools for building up "nano-QSAR": Quantitative features—property/activity relationships (QFPRs/QFARs). **In Book**: *J. Leszczynski, M.K. Shukla (Eds.)*. Practical Aspects of Computational Chemistry IV. Springer **2016**, pp. 353-396. DOI: 10.1007/978-1-4899-7699-4_12

- Toropov A.A., Toropova A.P. The CORAL software as spyglass to detect "coral reefs" in ocean of nanotechnologies. **2015**. *Available on the Atlas of Science* website: http://atlasofscience.org/the-coral-software-as-spyglass-to-detect-coral-reefs-in-ocean-of-nanotechnologies/#more-1267

- A.A. Toropov, A. P. Toropova, E. Benfenati, O. Nicolotti, A. Carotti, K. Nesmerak, A. M.Veselinovic, J. B. Veselinovic, P. R. Duchowicz, D. Bacelo, E. A. Castro, B. F. Rasulev, D. Leszczynska, J. Leszczynski,
***Chapter 15***. QSPR/QSAR analyses by means of the CORAL software: results, challenges, perspectives. **In Book**: *Roy, K. (Eds.)* Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment. **2015**, pp. 1-531. Hershey, PA: IGI Global. doi:10.4018/978-1-4666-8136-1 http://www.igi-global.com/book/quantitative-structure-activity-relationships-drug/120080

## Articles in Impacted (or Peer-reviewed) Journals

**2024:**

1. Alla P. Toropova and Andrey A. Toropov, The coefficient of conformism of a correlative prediction (CCCP): Building up reliable nano-QSPRs/QSARs for endpoints of nanoparticles in different experimental conditions encoded via quasi-SMILES. Science of the Total Environment 927 (2024) 172119. https://doi.org/10.1016/j.scitotenv.2024.172119
2. Alla P. Toropova, João Meneses, Ernesto Alfaro-Moreno, Andrey A. Toropov, The system of self-consistent models based on quasi-SMILES as a tool to predict the potential of Nano-inhibitors of human lung carcinoma cell line A549 for different experimental conditions. Drug and Chemical Toxicology, Published online: 06 Feb 2023. https://doi.org/10.1080/01480545.2023.2174986
3. Toropova, A.P., Toropov, A.A., Raska, I., Raskova, M., Carbó-Dorca, R. The prediction of the retention time of pesticide based on the Monte Carlo method with the use of the vector of the ideality of correlation and correlation weights of local symmetry fragments. J Math Chem (2023) Published: 23 September 2023. https://doi.org/10.1007/s10910-023-01517-0
4. A.P. Toropova, A.A. Toropov, A. Roncaglioni, E. Benfenati, Does the accounting of the local symmetry fragments in quasi-SMILES improve the predictive potential of the QSAR models of toxicity towards tadpoles? Toxicology Mechanisms and Methods, Accepted March 15, 2024. https://doi.org/10.1080/15376516.2024.2332617

**2023:**

5. Toropov, A.A., Di Nicola, M.R., Toropova, A.P., Roncaglioni, A., Dorne, J.L.C.M., Benfenati, E. Quasi-SMILES: Self-consistent models for toxicity of organic chemicals to tadpoles. Chemosphere 312 (2023) 137224. https://doi.org/10.1016/j.chemosphere.2022.137224
6. Toropova A.P., Toropov A.A., Fjodorova N. *In Silico* Simulation of Impacts of Metal Nano-Oxides on Cell Viability in THP-1 Cells Based on the Correlation Weights of the Fragments of Molecular Structures and Codes of Experimental Conditions Represented by Means of Quasi-SMILES. International Journal of Molecular Sciences, 24 (3), (2023) 2058. DOI: 10.3390/ijms24032058
7. Alla P. Toropova and Andrey A. Toropov, Quasi-SMILES as a basis to build up models of endpoints for nanomaterials. Environmental Technology, 44(28), 2023, 4460-4467. https://doi.org/10.1080/09593330.2022.2093655
8. Das, N.R., Sharma, T., Mallick, A., Toropova, A.P., Toropov, A.A., Achary, P.G.R. Computational Approach in Designing and Development of Novel Inhibitors of AKR1C1. Smart Innovation, Systems and Technologies, 2023, 317, 325–337. https://doi.org/10.1007/978-981-19-6068-0
9. Nilima R. Das, Tripti Sharma, Andrey A. Toropov, Alla P. Toropova, P. Ganga Raju Achary, Machine-Learning Technique, QSAR, and Molecular Dynamics for hERG-Drug Interactions. Journal of Biomolecular Structure & Dynamics, 41:23, (2023) 13766-13791. https://doi.org/10.1080/07391102.2023.2193641
10. A.P. Toropova, A.A. Toropov, A. Roncaglioni, E. Benfenati, Binding organophosphate pesticides to acetylcholinesterase: Risk assessment using the Monte Carlo method. Toxicological & Environmental Chemistry, 2023, 105:1-7, 19-27. DOI: 10.1080/02772248.2023.2181348
11. Andrey A. Toropov, Devon Barnes, Alla P. Toropova, Alessandra Roncaglioni, Alasdair R. Irvine, Rosalinde Masereeuw, Emilio Benfenati, CORAL models for drug induced nephrotoxicity. Toxics, 2023; 11(4): 293. https://doi.org/10.3390/toxics11040293
12. A.A. Toropov, A.P. Toropova, A. Roncaglioni, E. Benfenati, The system of self-consistent models for pesticide toxicity to *Daphnia Magna*, Toxicology Mechanisms and Methods, 2023, 33:7, 578-583. DOI: 10.1080/15376516.2023.2197487
13. A.P. Toropova, A.A. Toropov, A. Roncaglioni, E. Benfenati, D. Leszczynska, J. Leszczynski, CORAL: Model of ecological impact of heavy metals on soils via the study of modification of concentration of biomolecules in Earthworms (*Eisenia fetida*). Archives of Environmental Contamination and Toxicology, (2023) 84:504–515. https://doi.org/10.1007/s00244-023-01001-5

14. A.P. Toropova, A.A. Toropov, A. Roncaglioni, E. Benfenati, The system of self-consistent models: QSAR analysis of drug-induced liver toxicity. Toxics, 2023; 11(5):419. https://doi.org/10.3390/toxics11050419
15. J. Meneses, M. González-Durruthy, E. Fernandez-de Gortari, A.P. Toropova, A.A. Toropov, E. Alfaro-Moreno. A Nano-QSTR model to predict nano-cytotoxicity: an approach using human lung cells data. Particle and Fibre Toxicology, (2023) 20:21. https://doi.org/10.1186/s12989-023-00530-0
16. A.A. Toropov, A.P. Toropova, A. Roncaglioni, E. Benfenati, Does the accounting of the local symmetry fragments in SMILES improve the predictive potential of the QSPR-model for Henry's law constants? Environmental Science: Advances, 2023, 2, 916 - 921. https://doi.org/10.1039/D3VA00012E
17. Nilima R. Das, Tripti Sharma, Anshuman Chandra,Vijay Kumar Goel, Andrey A. Toropov, Alla P. Toropova, P. Ganga Raju Achary, Isoprenylcysteine Carboxyl Methyltransferase Inhibitors: QSAR, Docking and Molecular Dynamics Studies. Journal of Molecular Structure, 1291, 2023, 135966. https://doi.org/10.1016/j.molstruc.2023.135966
18. A.A. Toropov, A.P. Toropova, P.G.R. Achary, Prediction of n-octanol-water partition coefficient of platinum (IV) complexes using correlation weights of fragments of local symmetry. Structural Chemistry, 34, 1517–1526 (2023). https://doi.org/10.1007/s11224-023-02197-x
19. A.A. Toropova, A.P. Toropova, D. Leszczynska, J. Leszczynski, Development of self-consistency models of anticancer activity of nanoparticles that were observed under different experimental conditions using quasi-SMILES. Nanomaterials, 2023, 13(12), 1852. https://doi.org/10.3390/nano13121852
20. Alla P. Toropova, Andrey A. Toropov, Alessandra Roncaglioni, Emilio Benfenati, The enhancement scheme for the predictive ability of QSAR: a case of mutagenicity. Toxicology in Vitro 91 (2023) 105629. https://doi.org/10.1016/j.tiv.2023.105629
21. A.P. Toropova, A.A. Toropov, A. Roncaglioni, E. Benfenati, D. Leszczynska, J. Leszczynski, The validation of predictive potential via the system of self-consistent models: the simulation of blood-brain barrier permeation of organic compounds. Journal of Molecular Modeling, 29 (2023) 218. https://doi.org/10.1007/s00894-023-05632-2
22. Alla P. Toropova, Andrey A. Toropov, Parvin Kumar, Ashwani Kumar, P. Ganga Raju Achary, Fragments of local symmetry in a sequence of amino acids: Does one can use for QSPR/QSAR of peptides? Journal of Molecular Structure 1293 (2023) 136300. https://doi.org/10.1016/j.molstruc.2023.136300
23. Andrey A. Toropov, Alla P. Toropova, Alessandra Roncaglioni, Emilio Benfenati, *In silico* prediction of the mutagenicity of nitroaromatic compounds using correlation weights of fragments of local symmetry. Mutation Research - Genetic Toxicology and Environmental Mutagenesis 891 (2023) 503684. https://doi.org/10.1016/j.mrgentox.2023.503684
24. Alla P. Toropova, Andrey A. Toropov, Natalja Fjodorova, QSAR and Nano-QSAR: What is the common? The case of fullerenes solubility. Inorganics 2023, 11, 344. https://doi.org/10.3390/inorganics11080344.
25. Toropova, A.P.; Toropov, A.A.; Roncaglioni, A.; Benfenati, E. Using the Correlation Intensity Index to Build a Model of Cardiotoxicity of Piperidine Derivatives. Molecules 2023, 28, 6587. https://doi.org/10.3390/molecules28186587
26. N. Fjodorova, M. Novič, K. Venko, B. Rasulev, M.T. Saçan, G. Tugcu, S.S. Erdem, A.P. Toropova, A.A. Toropov, Cheminformatic and Machine Learning Approaches to the Assessment of Aquatic Toxicity Profile of Fullerene Derivatives. Int. J. Mol. Sci. 2023, 24, 14160. https://doi.org/10.3390/ijms241814160
27. Toropov, A.A.; Toropova, A.P.; Roncaglioni, A.; Benfenati, E.; Leszczynska, D.; Leszczynski, J. The System of Self-Consistent Models: The Case of Henry's Law Constants. Molecules 2023, 28, 7231. https://doi.org/10.3390/molecules28207231

28. Toropov, A.A.; Toropova, A.P.; Roncaglioni, A.; Benfenati, E. Semi-Correlations for Building Up a Simulation of Eye Irritation. Toxics 2023, 11, 993. https://doi.org/10.3390/toxics11120993
29. Alla P. Toropova and Andrey A. Toropov, Using the local symmetry in amino acids sequences of polypeptides to improve the predictive potential of models of their inhibitor activity. Amino Acids (2023) 55:1437–1445. DOI: 10.1007/s00726-023-03322-0

**2022:**

30. Alla P. Toropova, Andrey A. Toropov, Nanomaterials: quasi-SMILES as a flexible basis for regulation and environmental risk assessment. Science of the Total Environment 823 (2022) 153747. https://doi.org/10.1016/j.scitotenv.2022.153747
31. A.A. Toropov, F. Kjeldsen, A.P. Toropova, Use of quasi-SMILES to build models based on quantitative results from experiments with nanomaterials. Chemosphere 303 (2022) 135086. https://doi.org/10.1016/j.chemosphere.2022.135086
32. Alla P. Toropova, Andrey A. Toropov, Natalja Fjodorova, Quasi-SMILES for predicting toxicity of Nano-mixtures to *Daphnia Magna*. NanoImpact 28 (2022) 100427. https://doi.org/10.1016/j.impact.2022.100427
33. N. Fjodorova, M. Novič, K. Venko, V. Drgan, B. Rasulev, M. Türker Saçan, S. S. Erdem, G. Tugcu, A.P. Toropova, A.A. Toropov, How fullerene derivatives (FDs) act on therapeutically important targets associated with diabetic diseases. Computational and Structural Biotechnology Journal 20 (2022) 913–924. https://doi.org/10.1016/j.csbj.2022.02.006
34. Andrey A. Toropov, Alla P. Toropova, Valentin O. Kudyshkin, The system of self-consistent QSPR-models for refractive index of polymers. Structural Chemistry (2022) 33:617–624. https://doi.org/10.1007/s11224-021-01875-y
35. Andrey A. Toropov, Matteo R. Di Nicola, Alla P. Toropova, Alessandra Roncaglioni, Edoardo Carnesecchi, Nynke I. Kramer, Antony J. Williams, Manuel E. Ortiz-Santaliestra, Emilio Benfenati, Jean-Lou C.M. Dorne, A regression-based QSAR-model to predict acute toxicity of aromatic chemicals in tadpoles of the Japanese brown frog (*Rana japonica*): Calibration, validation, and future developments to support risk assessment of chemicals in amphibians, Science of the Total Environment 830 (2022) 154795. https://doi.org/10.1016/j.scitotenv.2022.154795
36. Andrey A. Toropov, Alla P. Toropova, P. Ganga Raju Achary, Maria Raškova, Ivan Raška Jr. The searching for agents for Alzheimer's disease treatment via the system of self-consistent models. Toxicology Mechanisms and Methods, 32:7, (2022) 549-557. https://doi.org/10.1080/15376516.2022.2053918
37. A.P. Toropova, A.A. Toropov, A. Lombardo, G. Lavado, and E. Benfenati, Paradox of "ideal correlations": improved model for air half-life of persistent organic pollutants. Environmental Technology 2022, Vol. 43, No. 16, 2510-2515. DOI: 10.1080/09593330.2021.1882588
38. Giovanna J. Lavado, Diego Baderna, Edoardo Carnesecchi, Alla P. Toropova, Andrey A. Toropov, Jean Lou C.M. Dorne, Emilio Benfenati, QSAR models for soil ecotoxicity: development and validation of models to predict reproductive toxicity of organic chemicals in the collembola *Folsomia candida*. Journal of Hazardous Materials 423 (2022) 127236. https://doi.org/10.1016/j.jhazmat.2021.127236
39. A.P. Toropova, A.A. Toropov, A. Roncaglioni, E. Benfenati, The system of self-consistent models of vapour pressure. Chemical Physics Letters 790 (2022) 139354. https://doi.org/10.1016/j.cplett.2022.139354
40. K. Jafari, M.H. Fatemi, A.P. Toropova, A.A. Toropov, The development of nano-QSPR models for viscosity of nanofluids using the index of ideality of correlation and the correlation intensity index, Chemometrics and Intelligent Laboratory Systems 222 (2022) 104500. https://doi.org/10.1016/j.chemolab.2022.104500
41. Andrey A. Toropov, Alla P. Toropova, Aleksandar Veselinovic, Danuta Leszczynska, Jerzy Leszczynski, SARS-CoV Mpro inhibitory activity of aromatic disulfide compounds: QSAR model.

Journal of Biomolecular Structure and Dynamics, 2022, 40(2), 780-786. DOI: 10.1080/07391102.2020.1818627
42. A.P. Toropova, A.A. Toropov, E.L. Viganò, E. Colombo, A. Roncaglioni, E. Benfenati, Carcinogenicity Prediction Using the Index of Ideality of Correlation. SAR and QSAR in Environmental Research, 2022; 33(6), 419-428, DOI: 10.1080/1062936X.2022.2076736
43. G. Selvestrel, G.J. Lavado, A.P. Toropova, A.A. Toropov, D. Gadaleta, M. Marzo, D. Baderna, E. Benfenati, Monte Carlo Models for Sub-Chronic Repeated-Dose Toxicity: Systemic and Organ-Specific Toxicity. International Journal of Molecular Sciences, 2022, 23, 6615. https://doi.org/10.3390/ijms23126615
44. Alla P. Toropova, Andrey A. Toropov, Alessandra Roncaglioni, Emilio Benfenati, Monte Carlo technique to study of the adsorption affinity of azo dyes with applying new statistical criteria of the predictive potential. SAR and QSAR in Environmental Research, 33(8), 2022, 621-630. DOI: 10.1080/1062936X.2022.2104369
45. Nilima R. Das, Krishnendu Bera, Tripti Sharma, Alla P. Toropova, Andrey A. Toropov, P. Ganga Raju Achary, Computational approach for building QSAR models for inhibition of HIF-1A. Journal of the Indian Chemical Society, 99 (10), 2022, 100687. https://doi.org/10.1016/j.jics.2022.100687
46. Parvin Kumar, Rahul Singh, Ashwani Kumar, Alla P. Toropova, Andrey A. Toropov, Meena Devi, Sohan Lal, Jayant Sindhu, Devender Singh, Identifications of Good and Bad Structural Fragments of Hydrazone/2,5-Disubstituted-1,3,4-oxadiazole Hybrids with correlation intensity index and consensus modelling using Monte Carlo Based QSAR Studies. SAR and QSAR in Environmental Research, 33(9), 2022, 677-700. https://doi.org/10.1080/1062936X.2022.2120068
47. Rahul Singh, Parvin Kumar, Meena Devi, Sohan Lal, Ashwani Kumar, Jayant Sindhu, Alla P. Toropova, Andrey A. Toropov and Devender Singh, Monte Carlo Based QSGFEAR: Prediction of Gibb's Free Energy of Activation at Different Temperatures Using SMILES Based Descriptors. New J. Chem., 2022, 46, 19062–19072. https://doi.org/10.1039/D2NJ03515D
48. Benfenati, E., Roncaglioni, A., Iovine, N., Mazzucotelli, M., Marzo, M., Toropov, A., Toropova, A., Baldin, R., Ciacci, A., M., Sartori, L., Yang, C., Magdziarz, T., Hobocienski, B., Mostrag, A., 2022. Maintenance, update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0. EFSA supporting publication 2022: 19(12): EN-7635. 50 pp. doi:10.2903/sp.efsa.2022.EN-7635.

**2021:**

49. Andrey A. Toropov and Alla P. Toropova, Quasi-SMILES as a basis for the development of models for the toxicity of ZnO nanoparticles. Science of the Total Environment, 772 (2021) 145532. https://doi.org/10.1016/j.scitotenv.2021.145532
50. A.P. Toropova and A.A. Toropov, The system of self-consistent of models: a new approach to build up and validation of predictive models of the octanol/water partition coefficient for gold nanoparticles. Int. J. Environ. Res. 15(4), 2021, 709-722. DOI: 10.1007/s41742-021-00346-w
51. Alla P. Toropova, Maria Raškova, Ivan Raška Jr., Andrey A. Toropov, The sequence of amino acids as the basis for the model of biological activity of peptides. Theoretical Chemistry Accounts, 140, 15 (2021). https://doi.org/10.1007/s00214-020-02707-8
52. Andrey A. Toropov and Alla P. Toropova, The unreliability of the reliability criteria in the estimation of QSAR for skin sensitivity: a pun or a reliable law? Toxicology Letters, 340 (2021) 133–140. https://doi.org/10.1016/j.toxlet.2021.01.015
53. J.L.C.M. Dorne, J. Richardson, A. Livaniou, E. Carnesecchi, L. Ceriani, R. Baldin, S. Kovarich, M. Pavan, E. Saouter, F. Biganzoli, L. Pasinato, M. Zare Jeddi, T. P. Robinson, G.E.N. Kass, A.K.D. Liem, A.A. Toropov, A.P. Toropova, C. Yang, A. Tarkhov, N. Georgiadis, M.R. Di Nicola, A. Mostrag, H. Verhagen, A. Roncaglioni, E. Benfenati, A. Bassan. EFSA's OpenFoodTox:

An open source toxicological database on chemicals in food and feed and its future developments. Environment International 146 (2021) 106293.
54. Gadaleta, D., Marzo, M., Toropov, A.A., Toropova, A.P., Lavado, G., Escher, S., Dorne, J.-L., Benfenati, E., Integrated in silico models for the prediction of No-Observed-(Adverse)-Effect-Levels and Lowest-Observed-(Adverse)-Effect-Levels in rats for sub-chronic repeated dose toxicity. Chemical Research in Toxicology, 2021, 34, 2, 247–257. https://doi.org/10.1021/acs.chemrestox.0c00176
55. Benfenati, E., Roncaglioni, A., Carnesecchi, E., Mazzucotelli, M., Marzo, M., Toropov, A.A., Toropova, A.P., Baldin, R., Ciacci, A., Kovarich, S., Sartori, L., Yang, C., Magdziarz, T., Hobocienski, B., Mostrag, A., Maintenance, update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0. EFSA supporting publication 2021: 18(3): EN-6476. 46pp. doi:10.2903/sp.efsa.2021.EN-6476
56. A.P. Toropova, A.A. Toropov, A. Roncaglioni, E. Benfenati, The index of ideality of correlation improves the predictive potential of models of the antioxidant activity of tripeptides from frog skin (*Litoria rubella*). Computers in Biology and Medicine, 133 (2021) 104370. https://doi.org/10.1016/j.compbiomed.2021.104370
57. A.P. Toropova, A.A. Toropov, E. Benfenati, The self-organizing vector of atom-pairs proportions: use to develop models for melting points. Structural Chemistry (2021) 32: 967–971. https://doi.org/10.1007/s11224-021-01778-y
58. A.P. Toropova, A.A. Toropov, J. Leszczynski, N. Sizochenko, Using quasi-SMILES for the predictive modeling of the safety of 574 metal oxide nanoparticles measured in different experimental conditions. Environmental Toxicology and Pharmacology 86 (2021) 103665. DOI: 10.1016/j.etap.2021.103665
59. P.G.R. Achary, A. P. Toropova, A.A. Toropov, Prediction of the self-accelerating decomposition temperature of organic peroxides. Process Safety Progress, 2021; 40: e12189. https://doi.org/10.1002/prs.12189
60. A.A. Toropov, A.P. Toropova, M. Marzo, E. Carnesecchi, G. Selvestrel, E. Benfenati, Pesticides, Cosmetics, Drugs: identical and opposite influences of various molecular features as measures of endpoints similarity and dissimilarity. Molecular Diversity, 25, 1137–1144 (2021). DOI: 10.1007/s11030-020-10085-3
61. A.A. Toropov, A.P. Toropova, A. Lombardo, A. Roncaglioni, G. Lavado, E. Benfenati, The Monte Carlo method to build up models of the hydrolysis half-lives of organic compounds. SAR and QSAR in Environmental Research, 2021, 32:6, 463-471. DOI: 10.1080/1062936X.2021.1914156
62. A. Worachartcheewan, A.P. Toropova, A. A. Toropov, R. Pratiwi, V. Prachayasittikul, C. Nantasenamat, Interpretable SMILES-based QSAR model of inhibitory activity of sirtuins 1 and 2. Combinatorial Chemistry & High Throughput Screening, 24(8), 2021, 1217 – 1228. DOI: 10.2174/1386207323666200902141907
63. Alla P. Toropova and Andrey A. Toropov, Can the Monte Carlo method predict the toxicity of binary mixtures? Environmental Science and Pollution Research, (2021) 28: 39493–39500. https://doi.org/10.1007/s11356-021-13460-1
64. A.P. Toropova, A.A. Toropov, D. Leszczynska, J. Leszczynski, Application of quasi-SMILES to the model of gold-nanoparticles uptake in A549 cells. Computers in Biology and Medicine 136 (2021) 104720. https://doi.org/10.1016/j.compbiomed.2021.104720
65. Andrey A. Toropov, Alla P. Toropova, The system of self-consistent models for the uptake of nanoparticles in PaCa2 cancer cells. Nanotoxicology, 15:7, 2021, 995-1004. DOI:10.1080/17435390.2021.1951387
66. Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, The QSAR-search of effective agents towards coronaviruses applying the Monte Carlo method. SAR and QSAR in Environmental Research, 32(9), (2021) 689-698. DOI:10.1080/1062936X.2021.1952649

67. A.P. Toropova, A. A. Toropov, E. Benfenati, Semi-correlations as a tool to model for skin sensitization. Food and Chemical Toxicology 157 (2021) 112580. https://doi.org/10.1016/j.fct.2021.112580
68. Andrey A. Toropov, Alla P. Toropova, Alessandra Roncaglioni, Emilio Benfenati, The system of self-consistent semi-correlations as one of the tools of cheminformatics for design antiviral drugs. New Journal of Chemistry, 2021, 45, 20713 – 20720. DOI: 10.1039/d1nj03394h

**2020:**

69. Andrey A. Toropov, Alla P. Toropova, QSPR/QSAR: state-of-art, weirdness, the future. Molecules 2020, 25(6), 1292. https://doi.org/10.3390/molecules25061292
70. Andrey A. Toropov and Alla P. Toropova, Correlation Intensity Index: building up models for mutagenicity of silver nanoparticles. Science of the Total Environment 737 (2020) 139720.
71. A.P. Toropova, A.A. Toropov, D. Leszczynska, J. Leszczynski, How the CORAL software can be used to select compounds for treatment of neurodegenerative diseases? Toxicology and Applied Pharmacology 408 (2020) 115276.
72. Andrey A.Toropov, Alla P.Toropova, Marco Marzo, Emilio Benfenati, Use of the index of ideality of correlation to improve aquatic solubility model. Journal of Molecular Graphics and Modelling 96 (2020) 107525.
73. Alla P. Toropova, Pablo R. Duchowicz, Laura M. Saavedra, Eduardo A. Castro and Andrey A. Toropov, The use of the index of ideality of correlation to build up models for bioconcentration factor. Molecular Informatics, 2020, 39, 1900070.
74. E. Carnesecchi, A.A. Toropov, A.P. Toropova, N. Kramer, C. Svendsen, J.L. Dorne, E. Benfenati, Predicting acute contact toxicity of organic binary mixtures in honey bees (A. mellifera) through innovative QSAR models. Science of the Total Environment 704 (2020) 135302.
75. Alla P. Toropova, Andrey A. Toropov, Emilio Benfenati, QSAR-models, validation, and IIC-paradox for drug toxicity. International Journal of Quantitative Structure-Property Relationships (IJQSPR), 5(1), 2020, 22-43.
76. Alla P. Toropova, Andrey A. Toropov, Edoardo Carnesecchi, Emilio Benfenati, Jean Lou Dorne. The index of ideality of correlation: models for flammability of binary liquid mixtures. Chemical Papers, 2020, 74(2): 601-609.
77. M. Marzo, G.J. Lavado, F. Como, A.A. Toropov, A.P. Toropova, D. Baderna, C. Cappelli, A. Lombardo, C. Toma, M. Blázquez Sánchez, E. Benfenati, QSAR models for Biocides. The example of the prediction of *Daphnia Magna* acute toxicity. SAR and QSAR in Environmental Research, 31:3, 227-243, 2020.
78. Toropov, A.; Toropova, A. QSPR/QSAR: State-of-art, Weirdness, the Future. Preprints 2020, 2020010325 (DOI: 10.20944/preprints202001.0325.v1).
79. Alla P. Toropova, Andrey A. Toropov, Danuta Leszczynska, Jerzy Leszczynski, The index of ideality of correlation: models of flash points of ternary mixtures. New Journal of Chemistry, 2020, 44, 4858 – 4868. DOI: 10.1039/D0NJ00121J
80. Alla P. Toropova, Andrey A. Toropov, Edoardo Carnesecchi, Emilio Benfenati, Jean Lou Dorne, The using of the Index of Ideality of Correlation (*IIC*) to improve predictive potential of models of water solubility for pesticides. Environmental Science and Pollution Research (2020) 27: 13339–13347.
81. K. Jafari, M.H. Fatemi, A.P. Toropova, A.A. Toropov, Correlation Intensity Index (CII) as a criterion of predictive potential: applying to model thermal conductivity of metal oxide-based ethylene glycol nanofluids. Chemical Physics Letters, 2020, 754, 137614.
82. Andrey A. Toropov, Alla P. Toropova, The Monte Carlo Method as a tool to build up predictive QSPR/QSAR. Curr. Comput. Aided Drug Des. 2020, 16(3), 197 – 206.

83. Andrey A. Toropov, Alla P. Toropova, Edoardo Carnesecchi, Emilio Benfenati, Jean Lou Dorne, The Index of Ideality of Correlation and the variety of molecular rings as a base to improve model of HIV-1 protease inhibitors activity. Structural Chemistry, (2020) 31: 1441–1448.
84. Alla P. Toropova, **Editorial**- Medicinal Chemistry and Computational Chemistry: Mutual Influence and Harmonization. Mini-Reviews in Medicinal Chemistry, 2020, 20(14), 1320-1321. DOI: 10.2174/1389557520142006261636l4
85. G.J. Lavado, D. Gadaleta, C. Toma, A. Golbamaki, A.A. Toropov, A.P. Toropova, M. Marzo, D. Baderna, E. Benfenati, Zebrafish AC50 Modelling: (Q)SAR Models to Predict Developmental Toxicity in Zebrafish Embryo. Ecotoxicology and Environmental Safety, 202 (2020) 110936.
86. Claudia Ileana Cappelli, Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, Ecosystem ecology: models for acute toxicity of pesticides towards *Daphnia magna*. Environmental Toxicology and Pharmacology, 80 (2020) 103459.
87. Alla P. Toropova, Andrey A. Toropov, Extending of QSPR/QSAR-algorithms in order to apply to nanomaterials. MDPI AG in MOL2NET 2020, International Conference on Multidisciplinary Sciences, 6th edition session NANOBIOMATJND-02: JSU-NDSU Nanotech. & BioMaterials Science Workshop, Jackson & Fargo, USA, 2020. Published: 28 July 2020. DOI: 10.3390/mol2net-06-06890
88. Alla P. Toropova and Andrey A. Toropov, Fullerenes C60 and C70: a model for solubility by applying the correlation intensity index. Fullerenes, Nanotubes and Carbon Nanostructures, 2020; 28:11, 900-906.
89. Andrey A. Toropov, Natalia Sizochenko, Alla P. Toropova, Danuta Leszczynska, Jerzy Leszczynski, Advancement of predictive modeling of zeta potentials (ζ) in metal oxide nanoparticles with correlation intensity index (*CII*). Journal of Molecular Liquids, 317 (2020) 113929.
90. Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, QSAR model for pesticides toxicity to Rainbow Trout based on “ideal correlations”. Aquatic Toxicology 227 (2020) 105589.
91. A.A. Toropov, A.P. Toropova, V.O. Kudyshkin, N.I. Bozorov, S.Sh. Rashidova, Applying of the Monte Carlo technique to build up models of glass transition temperatures of diverse polymers. Structural Chemistry, (2020) 31:1739–1743.
92. A.A. Toropov, A.P. Toropova, E. Benfenati, “Ideal correlations” for the predictive toxicity to *Tetrahymena pyriformis*. Toxicology Mechanisms and Methods, 30(8), 2020, 605-610.
93. Shahin Ahmadi, Alla P. Toropova, and Andrey A. Toropov, Correlation Intensity Index: Mathematical modelling of cytotoxicity of metal oxide nanoparticles. Nanotoxicology, 2020, 14:8, 1118-1126. DOI: 10.1080/17435390.2020.1808252
94. A.A. Toropov, A.P. Toropova, G. Selvestrel, D. Baderna, E. Benfenati, Prediction of No Observed Adverse Effect Concentration for Inhalation toxicity: Monte Carlo approach. SAR and QSAR in Environmental Research, 31(12), 2020, 1-12.

**2019:**

95. Alla P. Toropova, Andrey A. Toropov, QSPR and nano-QSPR: what is the difference? Journal of Molecular Structure, 1182 (2019) 141-149.
96. Andrey A. Toropov, Alla P. Toropova, The Correlation Contradictions Index (*CCI*): building up reliable models of mutagenic potential of silver nanoparticles under different conditions using quasi-SMILES. Science of the Total Environment 681 (2019) 102–109.
97. A.A. Toropov, I. Raška Jr., A.P. Toropova, M. Raškova, A.M. Veselinović, J.B. Veselinović, The study of the Index of Ideality of Correlation As a new criterion of predictive potential of QSPR/QSAR-models. Science of the Total Environment 659 (2019) 1387–1394.
98. Jose Luis Velazquez Libera, Julio Caballero, Alla Toropova, Andrey Toropov, Estimation of 2D autocorrelation descriptors and 2D Monte Carlo descriptors as a tool to build up predictive

models for acetylcholinesterase (AChE) inhibitory activity. Chemometrics and Intelligent Laboratory Systems, 184 (2019) 14–21.
99. A.P. Toropova, A.A. Toropov, A.M. Veselinović, J.B. Veselinović, D. Leszczynska, J. Leszczynski, Semi-correlations combined with the index of ideality of correlation: A tool to build up model of mutagenic potential. Molecular and Cellular Biochemistry, 2019, Volume 452, Issue 1–2, pp. 133–140.
100. Andrey A. Toropov, Alla P. Toropova, Use of The Index of Ideality of Correlation to improve predictive potential for biochemical endpoints. Toxicology Mechanisms and Methods, 2019, 29:1, 43-52.
101. C. Toma, D. Gadaleta, A. Roncaglioni, A. A.Toropov, A.P. Toropova, M. Marzo, E. Benfenati, QSAR development for plasma protein binding: influence of the ionization state. Pharmaceutical Research, (2019) 36: 28.
102. Alla P. Toropova, Andrey A. Toropov, Does the index of ideality of correlation detect the better model correctly? Mol. Inf. 2019, 38, 1800157.
103. Mariya A. Toropova, Maria Raškova, Ivan Raška Jr., Alla P. Toropova, The Index of Ideality of Correlation (*IIC*): model for sweetness. Monatshefte für Chemie - Chemical Monthly (2019) 150: 617–623.
104. P.G.R. Achary, A.P. Toropova, A.A. Toropov, Combinations of graph invariants and attributes of simplified molecular input-line entry system (SMILES) to build up models for sweetness. Food Research International 122 (2019) 40–46.
105. A.A. Toropov, A.P. Toropova, E. Benfenati, The Index of Ideality of Correlation: QSAR model of acute toxicity for zebrafish (*Danio rerio*) embryo. International Journal of Environmental Research (2019) 13: 387–394.
106. A.A. Toropov, A.P. Toropova, D. Leszczynska, J. Leszczynski, "Ideal correlations" for biological activity of peptides. BioSystems 181 (2019) 51–57.
107. Alla P. Toropova, Andrey A. Toropov, Quasi-SMILES: Quantitative Structure - Activity Relationships to predict anti-cancer activity. Molecular Diversity (2019) 23: 403–412.
108. A.P. Toropova, A.A. Toropov, E. Benfenati, D. Leszczynska, J. Leszczynski, Virtual Screening of Anti-Cancer Compounds: Application of Monte Carlo Technique. Anti-Cancer Agents in Medicinal Chemistry, 19(2), 2019, 148 – 153.
109. A.P. Toropova, A.A. Toropov, E. Benfenati, Semi-correlations as a tool to build up categorical (active/inactive) model of $GABA_A$ receptor modulators activity. Structural Chemistry (2019) 30 (3): 853–861.
110. Andrey A. Toropov, Alla P. Toropova, Gianluca Selvestrel, Emilio Benfenati, Idealization of correlations between optimal SMILES-based descriptors and skin sensitization. SAR and QSAR in Environmental Research, 30(6), 2019, 447-455.
111. Alla P. Toropova, Andrey A. Toropov, The index of ideality of correlation: Improvement of models for toxicity to algae. Natural Product Research, 33(15), 2019, 2200-2207.
112. A.A. Toropov, A.P. Toropova, G. Raitano, E. Benfenati, CORAL: building up QSAR models for the chromosome aberration test. Saudi Journal of Biological Sciences, 26 (2019) 1101–1106.
113. Alla P. Toropova, Andrey A. Toropov, Emilio Benfenati, QSPR as a random event: solubility of fullerenes C[60] and C[70]. Fullerenes, Nanotubes and Carbon Nanostructures, 2019, 27:10, 816-821.
114. Andrey A. Toropov, Alla P. Toropova, QSAR as a random event: criteria of predictive potential for a chance model. Structural Chemistry, 30(5), 2019, 1677-1683.
115. Alla P. Toropova, Andrey A. Toropov, Marco Marzo, Sylvia E. Escher, Jean Lou Dorne, Nikolaos Georgiadis, Emilio Benfenati, Corrigendum to “The application of new HARD-descriptor available from the CORAL software to building up NOAEL models” [Food Chem. Toxicol. 112 (2018) 544–550]. Food and Chemical Toxicology 128 (2019) 146.

116. A.P. Toropova, A.A. Toropov, Corrigendum to "CORAL: Binary classifications (active/inactive) for drug-induced liver injury" [Toxicol. Lett. 268 (2017) (February) 51–57]. Toxicology Letters, 313, 2019, 205.
117. A.P. Toropova, A.A. Toropov, Corrigendum to "Hybrid optimal descriptors as a tool to predict skin sensitization in accordance to OECD principles" [Toxicol. Lett. 275 (June) (2017) 57–66]. Toxicology Letters, 313, 2019, 206.
118. Alla P. Toropova and Andrey A. Toropov, Applying of the Monte Carlo method for the prediction of behavior of peptides. Current Protein & Peptide Science (2019) 20(12): 1151 - 1157.
119. Alla P. Toropova and Andrey A. Toropov, Whether the Validation of the Predictive Potential of Toxicity Models is Solved Task? Current Topics in Medicinal Chemistry, 2019; 19(29): 2643 – 2657.

**2018:**

120. Alla P. Toropova and Andrey A. Toropov, CORAL: QSAR Models for Carcinogenicity of Organic Compounds for Male and Female Rats. Computational Biology and Chemistry, 72, 2018, 26–32.
121. A.A. Toropov, R. Carbó-Dorca, A.P. Toropova, Index of Ideality of Correlation: new possibilities to validate QSAR: a case study. Structural Chemistry, (2018) 29: 33–38.
122. A.P. Toropova, A.A. Toropov, M. Marzo, S.E. Escher, J.L. Dorne, N. Georgiadis, E. Benfenati. The application of new HARD-descriptor available from the CORAL software to building up NOAEL models. Food and Chemical Toxicology, 112 (2018) 544-550.
123. Alla P. Toropova, Andrey A. Toropov, CORAL: Monte Carlo method to predict endpoints for medical chemistry. Mini-Reviews in Medicinal Chemistry, 18(5), 2018, 382 - 391.
124. A.A. Toropov, A.P. Toropova, E. Benfenati, M. Salmona, Mutagenicity, Anticancer activity, and Blood brain barrier: Similarity and dissimilarity of molecular alerts. Toxicology Mechanisms and Methods, 28(5), 2018, 321-327.
125. A.A. Toropov, N. Sizochenko, A.A. Toropova, J. Leszczynski, Towards the Development Of General Nano-Quantitative Structure-Property Relationship (nano-QSPR) Models: Zeta Potentials of Metal Oxide Nanoparticles. Nanomaterials, 2018, 8(4), 243.
126. Alla P. Toropova, Andrey A. Toropov, **Guest Editorial Preface**: Special Issue on Applications of QSPR/QSAR in Toxicology, Ecology, and Drug Discovery: Problems and Solutions. International Journal of Quantitative Structure-Property Relationships, Volume 3, Issue 2, 2018.
127. Andrey A. Toropov, Alla P. Toropova, Application of the Monte Carlo method for building up models for octanol-water partition coefficient of platinum complexes. Chemical Physics Letters 701 (2018) 137–146.
128. A.A. Toropov, A.P. Toropova, E. Benfenati, J. L. Dorne, SAR for gastro-intestinal absorption and blood-brain barrier permeation of pesticides. Chemico-Biological Interactions, 290 (2018) 1–5.
129. Alla P. Toropova, Andrey A. Toropov, Sanija Begum, Patnala Ganga Raju Achary, Blood brain barrier and Alzheimer's disease: Similarity and dissimilarity of molecular alerts. Current Neuropharmacology, 2018, 16, 769-785.
130. A. Worachartcheewan, A. P. Toropova, A. A. Toropov, S. Siriwong, J. Prapojanasomboon, V. Prachayasittikul, C. Nanatasenamat, Quantitative structure–activity relationship study of betulinic acid derivatives against HIV using SMILES-based descriptor. Current Computer-Aided Drug Design, 2018; 14(2): 152-159.
131. A.P. Toropova, A.A. Toropov, E. Benfenati, D. Leszczynska, J. Leszczynski, Prediction of antimicrobial activity of large pool of peptides using quasi-SMILES. BioSystems, 169–170 (2018) 5–12.
132. A.A. Toropov, A.P. Toropova, L. Cappellini, E. Benfenati, E. Davoli, QSPR analysis of threshold of odor for the large number of heterogenic chemicals. Molecular Diversity, (2018) 22: 397–403.

133. A.M. Veselinović, A.A. Toropov, A.P. Toropova, D. Stanković-Đorđević and J.B. Veselinović, Design and development of novel antibiotics based on FtsZ inhibition - in silico studies. New Journal of Chemistry, 2018, 42, 10976-10982.
134. A.A. Toropov, A.P. Toropova, E. Benfenati, L. Diomede, M. Salmona, Use of Quasi-SMILES to model biological activity of "micelle-polymer" samples. Structural Chemistry (2018) 29: 1213–1223.
135. Caterina Leone, Elia E. Bertuzzi, Alla P. Toropova, Andrey A. Toropov, Emilio Benfenati. CORAL: predictive models for cytotoxicity of functionalized nanozeolites based on quasi-SMILES. Chemosphere, 210 (2018) 52-56.
136. Alla P. Toropova, Andrey A. Toropov, Emilio Benfenati, Sara Castiglioni, Renzo Bagnati, Alice Passoni, Ettore Zuccato, Roberto Fanelli. Quasi-SMILES as a tool to predict removal rates of pharmaceuticals and dyes in sewage. Process Safety and Environmental Protection, 118 (2018) 227-233.
137. Alla P. Toropova, Andrey A. Toropov, Danuta Leszczynska, Jerzy Leszczynski, The Index of Ideality of Correlation: Hierarchy of Monte Carlo models for Glass Transition Temperatures of Polymers. Journal of Polymer Research, (2018) 25: 221-227.
138. Alla P. Toropova, Andrey A. Toropov, Use of the Index of Ideality of Correlation to improve models of Eco-toxicity. Environmental Science and Pollution Research, (2018) 25: 31771–31775.
139. Sanija Begum, P. Ganga Raju Achary, Andrey A. Toropov, Alla P. Toropova, Simplified molecular-input line-entry system based quantitative structure–activity relationship (QSAR) models for Serotonin 3 (5-HT3) receptor. Indian Journal of Chemistry Section-B, 57B, 2018, 1322-1327.
140. Andrey A. Toropov and Alla P. Toropova, Predicting Cytotoxicity of 2-Phenylindole Derivatives Against Breast Cancer Cells Using Index of Ideality of Correlation. Anticancer Research 38: 6189-6194 (2018).
141. Alla Toropova; Andrey Toropov; Emilio Benfenati, Idealized correlations: prediction of solubility of fullerene in organic solvents, Published: 10 December 2018 by MDPI AG in MOL2NET 2018, International Conference on Multidisciplinary Sciences, 4th edition session WCUCW-02: West Coast University Capstone Workshop, WCU, Miami, USA, 2018 (doi: 10.3390/mol2net-04-05898)

**2017:**

142. Alla P. Toropova, Andrey A. Toropov, **Editorial. Special issue**: Impact of Drug Metabolism and its Relevance upon Drug Discovery, Current Drug Metabolism, 18(12) (2017) 1070.
143. A.P. Toropova, A.A. Toropov. Nano-QSAR in cell biology: Model of cell viability as a mathematical function of available eclectic data. Journal of Theoretical Biology 416 (2017) 113–118.
144. A.P. Toropova, A.A. Toropov. CORAL: Binary classifications (active/inactive) for drug-induced liver injury. Toxicology Letters, 268, 15 February 2017, 51–57.
145. V. Prachayasittikula, A. Worachartcheewana, A.P. Toropova, A.A. Toropov, V. Prachayasittikul, C. Nantasenamat. Large-scale classification of P-glycoprotein inh ibitors using SMILES-based descriptors. SAR and QSAR in Environmental Research, 28(1), 2017, 1–16.
146. A.P. Toropova, A.A. Toropov, D. Leszczynska, J. Leszczynski. CORAL and Nano-QFAR: Quantitative feature – activity relationships (QFAR) for bioavailability of nanoparticles (ZnO, CuO, $Co_3O_4$, and $TiO_2$). Ecotoxicology and Environmental Safety, 2017; 139, 404-407.
147. A.P. Toropova, A.A. Toropov. The index of ideality of correlation: A criterion of predictability of QSAR models for skin permeability? Science of the Total Environment 586 (2017) 466–472.
148. Aleksandar M. Veselinović, Dragan Velimorović, Biljana Kaličanin, Alla Toropova, Andrey Toropov, Jovana Veselinović. Prediction of Gas Chromatographic Retention Indices Based on Monte Carlo Method. Talanta 168 (2017) 257–262.

149. K. Bouhedjar, S. Manganelli, G. Gini, A. A. Toropov, A. P. Toropova, S. Ali-Mokhnache, D. Messadi, QSAR Modeling useful in Anti-Cancer Drug Discovery: Prediction of $^{V600}$EBRAF-Dependent P-ERK using Monte Carlo Method. (2017) J. Med. Chem. Toxicol. 2(1): 1- 6.
150. Alla P. Toropova, Andrey A. Toropov. Hybrid Optimal Descriptors as a Tool to Predict Skin Sensitization in accordance to OECD principles. Toxicology Letters, 275 (2017) 57-66.
151. Andrey A. Toropov, Alla P. Toropova, Marten Beeg, Marco Gobbi, Mario Salmona, QSAR model for Blood-Brain Barrier Permeation. Journal of Pharmacological and Toxicological Methods 88 (2017) 7–18.
152. Andrey A. Toropov, Alla P. Toropova. The index of ideality of correlation: a criterion of predictive potential of QSPR/QSAR models? Mutation Research - Genetic Toxicology and Environmental Mutagenesis, 819 (2017) 31–37.
153. A. A. Toropov, A. P. Toropova, M. Marzo, J.L. Dorne, N. Georgiadis, E. Benfenati, QSAR models for predicting acute toxicity of pesticides in rainbow trout using the CORAL software and EFSA's OpenFoodTox database. Environmental Toxicology and Pharmacology 53 (2017) 158–163.
154. Andrey A. Toropov, Alla P. Toropova, Francesca Como, Emilio Benfenati, Quantitative structure–activity relationship models for bee toxicity. Toxicological & Environmental Chemistry, 99: 7-8, 2017, 1117-1128.
155. Benfenati E., Como F., Manzo M., Gadaleta D., Toropov A. and Toropova A., 2017. Developing innovative in silico models with EFSA's OpenFoodTox database. EFSA supporting publication 2017: EN-1206. 19 pp. doi:10.2903/sp.efsa.2017.EN-1206
156. Mariya A. Toropova, Ivan Raska Jr, Alla P. Toropova, Maria Raskova. CORAL software: analysis of impacts of pharmaceutical agents upon metabolism via the optimal descriptors. Current Drug Metabolism. Vol. 18, No. 6, 500-510, 2017.
157. Karel Nesměrák, Andrey A. Toropov, Alla P. Toropova, Tugba Ertan-Bolelli, Ilkay Yildiz. QSAR of antimycobacterial activity of benzoxazoles by optimal SMILES-based descriptors. Med. Chem. Res. (2017) 26: 3203–3208.
158. A.P. Toropova, A.A. Toropov, M. Beeg, M. Gobbi, M. Salmona, Utilization of the Monte Carlo method to build up QSAR models for hemolysis and cytotoxicity of antimicrobial peptides. Current Drug Discovery Technologies, 14(4), 2017, 229-243.

**2016:**

159. P. Ganga Raju Achary, Sanija Begum, Alla P. Toropova, Andrey A. Toropov, A quasi-SMILES based QSPR Approach towards the prediction of adsorption energy of Ziegler - Natta catalysts for propylene polymerization. Materials Discovery, 5, August 2016, 22–28. http://dx.doi.org/10.1016/j.md.2016.12.003
160. Alla P. Toropova, Terry W. Schultz, Andrey A. Toropov, Building up a QSAR model for toxicity towards *Tetrahymena Pyriformis* by the Monte Carlo method: A case of benzene derivatives. Environmental Toxicology and Pharmacology, 42 (2016) 135–145.
161. Karel Nesměrák, Andrey A. Toropov, Alla P. Toropova, Model for electrochemical parameters for 4-(benzylsulfanyl)pyridines calculated from the molecular structure. Journal of Electroanalytical Chemistry 766 (2016) 24–29.
162. S. Manganelli, C. Leone, A.A. Toropov, A.P. Toropova, E. Benfenati, QSAR model for predicting cell viability of human embryonic kidney cells exposed to $SiO_2$ nanoparticles. Chemosphere, 144 (2016) 995-1001.
163. Alla P. Toropova, Andrey A. Toropov, Aleksandar M. Veselinović, Jovana B. Veselinović, Emilio Benfenati, Danuta Leszczynska, Jerzy Leszczynski, Nano-QSAR: Model of mutagenicity of fullerene as a mathematical function of different conditions. Ecotoxicology and Environmental Safety, 124 (2016) 32-36.

164. Alla P. Toropova, Andrey A. Toropov, Evolution of Optimal Descriptors: Solved, Unsolved, and Unsoluble Tasks. International Journal of Quantitative Structure-Property Relationships, 1 (2), 2016, 52-71.
165. Manganelli, S., Leone, C., Toropov, A.A., Toropova, A.P., Benfenati, E. QSAR model for cytotoxicity of silica nanoparticles on human embryonic kidney cells. Materials Today: Proceedings, 3(3), 2016; 847–854.
166. Jovana B. Veselinović, Aleksandar M. Veselinović, Alla P. Toropova, Andrey A. Toropov, The Monte Carlo technique as a tool to predict LOAEL. European Journal of Medicinal Chemistry, 116 (2016) 71-75.
167. Andrey A. Toropov, Alla. P. Toropova, Emilio Benfenati, Roberto Fanelli, QSAR as a random event: selecting of the molecular structure for potential anti-tuberculosis agents. Anti-Infective Agents, 2016, 14(1): 3 – 10.
168. Toropova, A.P., Toropov, A.A., Rallo, R., Leszczynska, D., and Leszczynski, J., Nano-QSAR: Genotoxicity of multi-walled carbon nanotubes. Int. J. Environ. Res., 10(1): 59-64, 2016.
169. Andrey A. Toropov, Alla P. Toropova, Sanija Begum, P. Ganga Raju Achary, Towards predicting the solubility of $CO_2$ and $N_2$ in different polymers using a Quasi-SMILES based QSPR approach. SAR and QSAR in Environmental Research 27(4) (2016) 293-301.
170. Alla P. Toropova, Andrey A. Toropov, Serena Manganelli, Caterina Leone, Diego Baderna, Emilio Benfenati, Roberto Fanelli, Quasi-SMILES as a tool to utilize eclectic data for predicting the behavior of nanomaterials. NANOIMPACT 1 (2016) 60–64.
171. Veselinović A.M., Veselinović J.B., Nikolić G.M., Toropova A.P., Toropov A.A., QSPR models for estimating retention in HPLC with the *p* solute polarity parameter based on the Monte Carlo method. Struct. Chem. (2016) 27: 821–828.
172. Alla P. Toropova, P.Ganga Raju Achary, Andrey A. Toropov. Quasi-SMILES for Nano-QSAR prediction of toxic effect of $Al_2O_3$ nanoparticles. Journal of Nanotoxicology and Nanomedicine, 1(1), 2016, 17-28.
173. Alla P. Toropova, Andrey A. Toropov. QSPR model for dispersibility of graphene in various solvents. Letters in Drug Design & Discovery, 13(6), 2016, 514-520.
174. Andrey A. Toropov, P. Ganga Raju Achary, Alla P. Toropova. Quasi-SMILES and nano-QFPR: The predictive model for zeta potentials of metal oxide nanoparticles. Chemical Physics Letters 660 (2016) 107–110.
175. A.A. Toropov, A. P. Toropova, L. Cappellini, E. Benfenati, E. Davoli. Odor Threshold prediction by means of the Monte Carlo method. Ecotoxicology and Environmental Safety 133 (2016) 390–394.
176. A. P. Toropova, A. A. Toropov, A. M. Veselinović, J. B. Veselinović, D. Leszczynska, J. Leszczynski, Monte Carlo based QSAR models for toxicity of organic chemicals to *Daphnia magna*. Environmental Toxicology and Chemistry, 2016; Vol. 35, No. 11, pp. 2691–2697.
177. Alla P. Toropova, Andrey A. Toropov, Maria Raskova, Ivan Raska Jr, Improved building up a model of toxicity towards *Pimephales promelas* by the Monte Carlo method. Environmental Toxicology and Pharmacology 48 (2016) 278–285.
178. Alla P. Toropova and Andrey A. Toropov, Assessment of nano-QSPR models of organic contaminant absorption by carbon nanotubes for ecological impact studies. Materials Discovery, 4 (2016) 22–28.
179. Bragazzi N, Toropov AA, Toropova AP, Pechkova E, Nicolini C. 2016. Quasi-QSPR to Predict Proteins Behavior Under Various Concentrations of Drug Using Nanoconductometric Assay. NanoWorld J. 2(4): 71-77. http://dx.doi.org/10.17756/nwj.2016-000

**2015:**

180. A. P. Toropova, A.A. Toropov, R. Rallo, D. Leszczynska, J. Leszczynski. Optimal descriptor as a translator of eclectic data into prediction of cytotoxicity for metal oxide nanoparticles under different conditions. Ecotoxicology and Environmental Safety, (2015) 112, 39–45.
181. A.A. Toropov and A.P. Toropova. Quasi-QSAR for mutagenic potential of multi-walled carbon-nanotubes. Chemosphere, (2015) 124: 40–46.
182. A.P. Toropova and A. A. Toropov. Mutagenicity: QSAR - quasi-QSAR - nano-QSAR. Mini-Reviews in Medicinal Chemistry, 2015, 15(2): 608-621.
183. Alla P. Toropova and Andrey A. Toropov, Quasi-SMILES and nano-QFAR: United model for mutagenicity of fullerene and MWCNT under different conditions. Chemosphere, 139 (2015) 18–22.
184. Andrey A. Toropov and Alla P. Toropova, **Editorial**. Special issue: "From Chemoinformatics to Nanoinformatics: New tools for Drug Discovery and Nanoparticles Design in Medicinal Chemistry", Current Topics in Medicinal Chemistry, 2015 May 6, 15(18) 1767.
185. A. P. Toropova, A. A. Toropov, J. B. Veselinović, A. M. Veselinović. QSAR as a random event: a case of NOAEL. Environ. Sci. Poll. Res. (2015), 22(11), 8264-8271
186. J. B. Veselinovic´, A. A. Toropov, A. P. Toropova, G. M. Nikolic´, A. M. Veselinovic´. Monte Carlo Method-Based QSAR Modeling of Penicillins Binding to Human Serum Proteins. Arch. Pharm. (2015) 348 (1), 62-67.
187. P.R. Duchowicz, S.E. Fioressi, D.E. Bacelo, L.M. Saavedra, A.P. Toropova, A.A. Toropov, QSPR Studies on Refractive Indices of Structurally Heterogeneous Polymers. Chemom. Intell. Lab. Syst., (2015) 140, 86–91.
188. A.P. Toropova, A.A. Toropov, E. Benfenati, R. Korenstein, D. Leszczynska, J. Leszczynski. Optimal nano-descriptors as translators of eclectic data into prediction of the cell membrane damage by means of nano metal-oxides. Environ. Sci. Pollut. Res. (2015) 22, 745–757.
189. A.A. Toropov, J. B. Veselinovic´, A. M. Veselinovic´, F. N. Miljkovic´, A. P. Toropova, QSAR models for 1, 2, 4-benzotriazines as Src inhibitors based on Monte Carlo method. Med. Chem. Res. (2015) 24 (1), 283-290
190. Toropova A.P., Toropov A.A., Benfenati E. A quasi-QSPR modeling for the photocatalytic decolorisation rate constants and cellular viability (CV%) of nanoparticles by CORAL. SAR and QSAR in Environmental Research, Jan 2015, 26(1); 29-40.
191. A.M. Veselinović, J. B. Veselinović, A.A. Toropov, A.P. Toropova, G. M. Nikolić. QSAR Models for the Reactivation of Sarin Inhibited AChE by Quaternary Pyridinium Oximes Based on Monte Carlo Method. Current computer-aided drug design, 2015, 10(3), 266-273.
192. A.P. Toropova, A.A. Toropov, E. Benfenati, D. Leszczynska, J. Leszczynski. QSAR model as a random event: A case of rat toxicity. Bioorganic & Medicinal Chemistry, 2015, 23(6), 1223-1230.
193. Andrey A. Toropov, Alla P. Toropova, Claudia Ileana Cappelli, Emilio Benfenati. CORAL: model for octanol/water partition coefficient. Fluid Phase Equilibria, (2015); 397, 44-49.
194. A.A. Toropov, A. P. Toropova, A. M. Veselinović, J. B. Veselinović, K. Nesměrák, I. Raska Jr, P. R. Duchowicz, E. A. Castro,V. O. Kudyshkin, D. Leszczynska, J. Leszczynski. The Monte Carlo method based on eclectic data as an efficient tool for predictions of endpoints for nanomaterials – two examples of application. Combinatorial Chemistry & High Throughput Screening. 2015, 18(4), 376-386.
195. Alla P. Toropova, Andrey A. Toropov, Valentin O. Kudyshkin, Robert Rallo, Prediction of the Q-e parameters from structures of transfer chain agents, Journal of Polymer Research, 22 (2015)128.
196. Andrey A. Toropov, Robert Rallo, Alla P. Toropova, Use of quasi-SMILES and Monte Carlo optimization to develop quantitative feature property/activity relationships (QFPR/QFAR) for nanomaterials. Current Topics in Medicinal Chemistry, 2015, 15(18) 1837-1844.

197. Andrey A. Toropov, Alla P. Toropova, Fabiola Pizzo, Anna Lombardo, Domenico Gadaleta, Emilio Benfenati. CORAL: Model for No Observed Adverse Effect Level (NOAEL). Molecular Diversity, 19(3) (2015) 563-575.
198. A.P. Toropova, A.A. Toropov, and E. Benfenati, CORAL: Prediction of binding affinity and efficacy of thyroid hormone receptor ligands. Eur. J. Med. Chem., 101 (2015) 452-461.
199. Apilak Worachartcheewan, Virapong Prachayasittikul, Alla P. Toropova, Andrey A. Toropov, Chanin Nantasenamat, Large-scale structure-activity relationship study of hepatitis C virus NS5B polymerase inhibition using SMILES-based descriptors. Molecular Diversity, 19 (2015) 955–964.
200. A.M. Veselinović, J. B. Veselinović, A. A. Toropov, A. P. Toropova, G. M. Nikolić; In Silico Prediction of the $\beta$-Cyclodextrin Complexation Based on Monte Carlo Method. International Journal of Pharmaceutics, 2015 Aug 28; 495(1): 404-409.
201. A. P. Toropova, A. A. Toropov, J.B. Veselinović, A. M. Veselinović, E. Benfenati, D. Leszczynska, J. Leszczynski. Application of the Monte Carlo method to prediction of dispersibility of graphene in various solvents. Int. J. Environ. Res., 9 (4): 1211-1216, 2015.
202. Karel Nesměrák , Andrey A. Toropov, Alla P. Toropova, Ilkay Yildiz, Ismail Yalcin, Marketa Brozikova, Vera Klimešová, Karel Waisser, Prediction of Retention Characteristics of Heterocyclic Compounds. Analytical and Bioanalytical Chemistry, (2015) 407: 9185–9189.
203. Toropova, A.; Toropov, A. CORAL: The dispersion of SWNTs in different organic solvents. In Proceedings of the MOL2NET, 5–15 December 2015; Sciforum Electronic Conference Series, Vol. 1, 2015, c007; doi:10.3390/MOL2NET-1-c007

**2014:**

204. Toropov A. A., Toropova A. P., Raska I. Jr., Leszczynska D., Leszczynksy J., Comprehension of drug toxicity: Software and databases. Computers in Biology and Medicine, (2014); 45: 20-25
205. Toropova A.P., Toropov A. A., CORAL software: Prediction of Carcinogenicity of Drugs by means of The Monte Carlo method. European Journal of Pharmaceutical Sciences, (2014); 52: 21-25
206. Toropov A. A., Toropova A. P., Optimal descriptor as a translator of eclectic data into endpoint prediction: Mutagenicity of fullerene as a mathematical function of conditions. Chemosphere (2014); 104: 262-264
207. J. Veselinović, A. Veselinović, A. Toropov, A. Toropova, I.Damnjanović, G. Nikolić, Monte Carlo Method Based QSAR Modeling of Coumarin Derivates as Potent HIV-1 Integrase Inhibitors and Molecular Docking Studies of Selected 4-phenyl Hydroxycoumarins. Scientific Journal of the Faculty of Medicine in Niš (2014); 31(2): 95-103
208. A.P. Toropova, A.A. Toropov, J. B. Veselinović, F.N. Miljković, A. M. Veselinović, QSAR models for HEPT derivates as NNRTI inhibitors based on Monte Carlo method. European Journal of Medicinal Chemistry, (2014); 77: 298–305
209. Nesměrák K., Toropov A.A, Toropova A.P. SMILES-based quantitative structure-retention relationships for RP-HPLC of 1-phenyl-5-benzylsulfanyltetrazoles. Structural Chemistry, (2014); 25: 311–317
210. Nieves C. Comelli, Erlinda V. Ortiz, Magdalena Kolacz, Alla P. Toropova, Andrey A. Toropov, Pablo R. Duchowicz, Eduardo A. Castro, Conformation-Independent QSAR on c-Src Tyrosine Kinase Inhibitors. Chemometrics and Intelligent Laboratory Systems, (2014) 134: 47–52.
211. Toropov A. A., Toropova A. P., Kudyshkin V. O., Leszczynska D., Leszczynksy J., Optimal descriptors as a tool to predict the thermal decomposition of polymers, Journal of Mathematical Chemistry, (2014); 52:1171–1181.

212. Worachartcheewan A., Mandi P., Prachayasittikul V., Toropova A.P., Toropov A.A., Nantasenamat C. Large-scale QSAR study of aromatase inhibitors using SMILES-based descriptors. Chemometrics and Intelligent Laboratory Systems, (2014) 138, 120-126.
213. Karthick V., Toropova A.P., Toropov A.A., Ramanathan K. Discovery of potential, non-toxic influenza virus inhibitor by computational techniques. Molecular Informatics, (2014) 33 (8), 559-565.
214. Toropova A. P., Toropov A. A., Benfenati E., Puzyn T., Leszczynska D., Leszczynksy J. Optimal descriptor as a translator of eclectic information into the prediction of membrane damage: the case of a group of ZnO and $TiO_2$ nanoparticles. Ecotoxicology and Environmental Safety (2014); 108, 203–209.
215. Vijay H. Masand, Andrey A. Toropov, Alla P. Toropova, Devidas T. Mahajan, QSAR models for anti-malarial activity of 4-aminoquinolines. Current Computer-Aided Drug Design, (2014), 10: 75-82.
216. Gissi A., Toropov A.A., Toropova A.P., Nicolotti O., Carotti A., Benfenati E. Building up QSAR model for toxicity of psychotropic drugs by the Monte Carlo method, Structural Chemistry, (2014); 25: 1067-1073.
217. Toropova A.P., Toropov A.A., Benfenati E., Korenstein R. QSAR model for cytotoxicity of $SiO_2$ nanoparticles on human lung fibroblasts, J. Nanopart. Res. (2014); 16: 2282.

**2013:**

218. Toropov A. A., Toropova A. P., Raska I. Jr., Benfenati E., Gini G. Development of QSAR models for predicting anti-HIV-1 activity using the Monte Carlo method. Central European Journal Chemistry 2013; 11: 371-380.
219. Toropov A. A., Toropova A. P., Benfenati E., Gini G., Leszczynska D., Leszczynksy J. CORAL: QSPR model of water solubility based on local and global SMILES attributes. Chemosphere, 2013; 90: 877-880.
220. Toropov A. A., Toropova A. P., Benfenati E., Gini G., Leszczynska D., Leszczynksy J., De Nucci G. QSAR models for inhibitors of physiological impact of Escherichia coli that leads to diarrhea. Biochem. Biophys. Res. Commun, 2013; 432: 214-225.
221. Toropova A. P., Toropov A. A., Martyanov S. E., Benfenati E., Gini G., Leszczynska D., Leszczynksy J. CORAL: Monte Carlo method as a tool for the prediction of the bioconcentration factor of industrial pollutants. Mol. Inform. 2013; 32 : 145-154.
222. Toropov A. A., Toropova A. P., Puzyn T., Benfenati E., Gini G., Leszczynska D., Leszczynksy J., QSAR as a random event: Models for nanoparticles uptake in PaCa2 cancer cells. Chemosphere, 2013; 92: 31–37.
223. Toropov A.A., Toropova A.P., Benfenati E., Gini G.: OCWLGI Descriptors: Theory and Praxis, Current Computer-Aided Drug Design 2013; 9: 226-232.
224. A.P. Toropova, A.A. Toropov, E. Benfenati, G. Gini, D. Leszczynska, J. Leszczynski: CORAL: QSPRs of enthalpies of formation of organometallic compounds, J. Math. Chem 2013; 51: 1684-1693.
225. Nesměrák K., Toropov A.A, Toropova A.P., Kohoutova P., Waisser K., SMILES-based quantitative structure-property relationships for half-wave potential of N-benzylsalicyl thioamides. European Journal of Medicinal Chemistry, 2013, 67: 111-114.
226. A.A. Toropov, A.P. Toropova , E. Benfenati, G. Gini, R. Fanelli, The definition of the molecular structure for potential anti-malaria agents by the Monte Carlo method. Struct. Chem, 2013; 24:1369–1381

A. Roncaglioni, A.A. Toropov, A.P. Toropova, E. Benfenati, In silico methods to predict drug toxicity. Current Opinion in Pharmacology, 2013; 13: 802–806.

227. A.P. Toropova, A.A. Toropov, T. Puzyn, E. Benfenati, D. Leszczynska, J. Leszczynski, Optimal descriptor as a translator of eclectic information into the prediction of thermal conductivity of Micro-Electro-Mechanical Systems. J. Math. Chem. 2013; 51: 2230-2237
228. A.P. Toropova, A. A. Toropov, Optimal descriptor as a translator of eclectic information into the prediction of membrane damage by means of various $TiO_2$ nanoparticles. Chemosphere, 2013; 93: 2650–2655.

**2012:**

229. Toropova AP, Toropov AA, Rasulev B, Benfenati E, Gini G, Leszczynska D, Leszczynksy J, QSAR models for ACE-inhibitor activity of tri-peptides based on representation of the molecular structure by a graph of atomic orbitals and SMILES. Structural Chemistry, 23 (2012) 1873-1878
230. Toropov AA, Toropova AP, Benfenati E, Gini G, Leszczynska D, Leszczynksy J. CORAL: Classification model for predictions of anti-sarcoma activity. Curr .Top. Med. Chem. 2012; 12: 2741-2744.
231. Toropov AA, Toropova AP, Raska I Jr, Benfenati E, Gini G, QSAR modeling of endpoints for peptides which is based on representation of the molecular structure by a sequence of amino acids. Structural Chemistry 23 (2012) 1891-1904.
232. Toropova A P, Toropov A A, Benfenati E, Gini G, Leszczynska D, Leszczynksy J. CORAL: Models of toxicity of binary mixtures. Chemometrics Intelligent Laboratory System 119 (2012) 39-43.
233. A.A. Toropov, A.P. Toropova, B.F. Rasulev, E. Benfenati, G. Gini, D. Leszczynska, J. Leszczynski, CORAL: Binary Classifications (Active/Inactive) for Liver-Related Adverse Effects of Drugs. Current Drug Safety, 7 (2012) 257-261.
234. A.A.Toropov, A.P. Toropova, E. Benfenati, G. Gini, D. Leszczynska, J. Leszczynski, Calculation of molecular features with apparent impact on both activity of mutagens and activity of anticancer agents. Anti-Cancer Agents in Med. Chem. 12 (2012) 807-817.
235. A.A. Toropov, A.P. Toropova, E. Benfenati, G. Gini, T. Puzyn, D. Leszczynska, J. Leszczynski, Novel application of the CORAL software to model cytotoxicity of metal oxide nanoparticles to bacteria *Escherichia coli*. Chemosphere 89 (2012) 1098–1102
236. A.P. Toropova, A.A. Toropov, E. Benfenati, G. Gini, D. Leszczynska, J. Leszczynski, Coral: Quantitative model for estimating bioconcentration factor of organic compounds. Chemometr. Intell. Lab. 118 (2012)70-73
237. A.A. Toropov, A.P. Toropova, B.F. Rasulev, E. Benfenati, G. Gini, D. Leszczynska, J. Leszczynski, Coral: QSPR Modeling of Rate Constants of Reactions Between Organic Aromatic Pollutants and Hydroxyl Radical, J. Comput. Chem. 33 (2012) 1902-1906.
238. A.A. Toropov, A.P. Toropova, A. Lombardo, A. Roncaglioni, N. De Brita, G. Stella, E. Benfenati, CORAL: the prediction of biodegradation of organic compounds with optimal SMILES-based descriptors, Cent. Eur. J. Chem. 10 (2012) 1042-1048
239. A.P. Toropova, A.A. Toropov, E. Benfenati, G. Gini, D. Leszczynska, J. Leszczynski, The average numbers of outliers over groups of various splits into training and test sets: A criterion of the reliability of a QSPR? A case of water solubility, Chemical Physics Letters 542 (2012) 134-137.
240. A.P. Toropova, A.A. Toropov, A. Lombardo, A. Roncaglioni, E. Benfenati, G.Gini, CORAL: QSAR model for acute toxicity in Fathead Minnow (*Pimephales promelas*). J. Comput. Chem. 33(2012)1218-1223
241. A.P. Toropova, A.A. Toropov, S.E. Martyanov, E. Benfenati, G.Gini, D. Leszczynska, J. Leszczynski, CORAL: QSAR modeling of toxicity of organic chemicals towards Daphnia magna, Chemometr. Intell. Lab. 110(2012)177-181.
242. Toropova AP, Toropov AA, Benfenati E, Gini G., QSAR models for toxicity of organic substances to *Daphnia magna* built up by using the CORAL freeware. Chem. Biol. Drug. Des. 79 (2012): 332-338.

243. Toropov AA, Toropova AP, Martyanov SE, Benfenati E, Gini G, Leszczynska D, Leszczynksy J. CORAL: Predictions of rate constants of hydroxyl radical reaction using representation of the molecular structure obtained by combination of SMILES and Graph approaches. Chemometrics Intelligent Laboratory System 112 (2012): 65-70.
244. Toropov AA, Toropova AP, Gonella Diaza R, Benfenati E, Gini G. SMILES-based optimal descriptors: QSAR modeling of estrogen receptor binding affinity by correlation balance. Structural Chemistry 23 (2012) 529-544.

**2011:**

245. A.A. Toropov, A.P. Toropova, E. Benfenati, G. Gini, D. Leszczynska, J. Leszczynski, SMILES-based QSAR approaches for carcinogenicity and anticancer activity: Comparison of correlation weights for identical SMILES attributes. Anti-cancer. Agents. Med. Chem. 11 (2011) 974-982.
246. A.A. Toropov, A.P. Toropova, S.E. Martyanov, E. Benfenati, G. Gini, D. Leszczynska, J. Leszczynski, Comparison of SMILES and molecular graphs as the representation of the molecular structure for QSAR analysis for mutagenic potential of polyaromatic amines. Chemometr. Intell. Lab. 109 (2011) 94-100.
247. A.P. Toropova, A. A. Toropov, E. Benfenati, G. Gini, D. Leszczynska, J. Leszczynski, QSAR modeling of anxiolytic activity taking into account the presence of keto- and enol-tautomers by balance of correlations with ideal slopes. Cent. Eur. J. Chem. 9(5) (2011) 846-854.
248. A.P. Toropova, A.A. Toropov, E. Benfenati, G. Gini, D. Leszczynska, J. Leszczynski, CORAL: Quantitative Structure–Activity Relationship Models for Estimating Toxicity of Organic Compounds in Rats, J. Comput. Chem. 32 (2011) 2727-2733.
249. A.P. Toropova, A.A. Toropova, E. Benfenati, G. Gini, QSAR modelling toxicity toward rats of inorganic substances by means of CORAL. Cent. Eur. J. Chem. 9(1) (2011) 75-85.
250. Toropova, A.P., Toropov, A.A., Benfenati, E., Gini, G., Leszczynska, D., Leszczynski, J. CORAL: QSPR models for solubility of [$C_{60}$] and [$C_{70}$] fullerene derivatives. Mol. Divers 105(2011)249-256.
251. A.P. Toropova, A.A. Toropov, R. Gonella Diaza, E. Benfenati, G. Gini, Analysis of the co-evolutions of correlations as a tool for QSAR-modeling carcinogenicity: an unexpected good prediction based on a model that seems untrustworthy. Cent. Eur. J. Chem 9(2011) 165-174
252. A.P. Toropova, A.A. Toropov, E. Benfenati, G. Gini, Co-evolutions of correlations for QSAR of toxicity of organometallic and inorganic substances: an unexpected good prediction based on a model that seems untrustworthy. Chemometr. Intell. Lab. 105 (2011) 215-219.
253. A.A. Toropov, A.P. Toropova, A. Lombardo, A. Roncaglioni, E. Benfenati, G. Gini CORAL: building up the model for bioconcentration factor and defining it's applicability domain. Eur. J. Med. Chem. 46 (2011) 1400-1403.
254. A.P. Toropova, A,A. Toropov, E. Benfenati, G. Gini, Simplified Molecular Input-Line Entry System and International Chemical Identifier in the QSAR Analysis of Styrylquinoline Derivatives as HIV-1 Integrase Inhibitors. Chem. Biol. Drug Des. 77 (2011) 343-360
255. E. Benfenati, A.A. Toropov, A.P. Toropova, A. Manganaro, R. Gonella Diaza, CORAL software: QSAR for anticancer Agents. Chem. Biol. Drug Des. 77(2011) 471-476

**2010:**

256. A.A. Toropov, A.P. Toropova and E. Benfenati, QSAR modelling of the toxicity to *Tetrahymena pyriformis* by balance of correlations. Mol. Divers. 14 (2010) 821-827
257. A.A. Toropov, A.P. Toropova and E. Benfenati, QSPR modeling of normal boiling points and octanol/water partition coefficient for acyclic and cyclic hydrocarbons using SMILES based optimal descriptors. Cent. Eur. J. Chem. 8 (2010) 1047-1052.

258. Alla P. Toropova, Andrey A. Toropov, Emilio Benfenati, Danuta Leszczynska, Jerzy Leszczynski, QSAR modeling of measured binding affinity for fullerene-based HIV-1 PR inhibitors by CORAL. J. Math. Chem. 47 (2010) .959-987.
259. Toropov A.A., Toropova A.P., Benfenati E., Leszczynska D., Leszczynski J., SMILES-Based Optimal Descriptors: QSAR Analysis of Fullerene-Based HIV-1 PR Inhibitors by Means of Balance of Correlations. J. Comput. Chem. 31 (2010) 381-392.
260. Toropov A.A., Toropova A.P., Benfenati E., Leszczynska D., Leszczynski J. InChI-based optimal descriptors: QSAR analysis of fullerene [C60]-based HIV-1 PR inhibitors by correlation balance. European Journal of Medicinal Chemistry 45 (2010) 1387–1394.
261. A.A. Toropov, A. P. Toropova, I. Raska , E. Benfenati, QSPR modeling of octanol/water partition coefficient of antineoplastic agents by balance of correlations. European Journal of Medicinal Chemistry 45 (2010) 1639–1647.
262. Toropov A.A., Toropova A.P., Benfenati E. QSAR-modeling of toxicity of organometallic compounds by means of the balance of correlations for InChI-based optimal descriptors. Mol. Divers. 14 (2010) 183-192.
263. A.A. Toropov, A. P. Toropova, E. Benfenati, D. Leszczynska, J. Leszczynski, QSAR analysis of 1,4-dihydro-4-oxo-1-(2-thiazolyl)- 1,8-naphthyridines exhibiting anticancer activity by optimal SMILES-based descriptors. J. Math. Chem. 47 (2010) 647–666.
264. Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, Danuta Leszczynska, Jerzy Leszczynski, Use of the international chemical identifier for constructing QSPR-model of normal boiling points of acyclic carbonyl substances. J. Math. Chem. 47 (2010) 355–369
265. A.A. Toropov, A.P. Toropova, E. Benfenati, SMILES-based optimal descriptors: QSAR modelling of carcinogenicity by balance of correlations with ideal slopes. Eur. J. Med. Chem. 45 (2010) 3581-3587.
266. A.P. Toropova, A.A. Toropov, A. Lombardo, A. Roncaglioni E. Benfenati, G. Gini, A new model for bioconcentration factor based on SMILES and Indices of presence of atoms. Eur. J. Med. Chem. 45 (2010) 4399-4402

**2009:**

267. Toropov A.A., Toropova A.P., Benfenati E. QSPR modeling of octanol water partition coefficient of platinum complexes by InChI-based optimal descriptors. J. Math. Chem. 46 (2009) 1060-1073
268. Toropov A.A., Toropova A.P., Benfenati E. Leszczynska, D., Leszczynski, J.; Additive InChI-based optimal descriptors: QSPR modeling of fullerene C60 solubility in organic solvents. J. Math. Chem. 46 (2009) 1232-1251
269. Toropov A.A., Toropova A.P., Benfenati E., Manganaro, A. QSAR modelling of carcinogenicity by balance of correlations. Molecular Diversity, 2009, pp. 397-404
270. Toropov A.A., Toropova A.P., Benfenati E. QSPR modeling bioconcentration factor (BCF) by balance of correlations. European Journal of Medicinal Chemistry, (2009) 44 (6), 2544-2551.
271. Toropov A.A.; Toropova, A.P.; Benfenati, E. Additive SMILES-Based Carcinogenicity Models: Probabilistic Principles in the Search for Robust Predictions. Int. J. Mol. Sci. 2009, 10, 3106-3127.
272. Toropov A.A., Toropova A.P., Benfenati, E. Simplified molecular input line entry system-based optimal descriptors: Quantitative structure-activity relationship modeling mutagenicity of nitrated polycyclic aromatic hydrocarbons. Chemical Biology and Drug Design, (2009) 73 (5), pp. 515-525.
273. Toropov A.A., Toropova A.P., Benfenati E. QSPR modelling of the octanol/water partition coefficient of organometallic substances by optimal SMILES-based descriptors. Central European Journal of Chemistry, (2009) 7 (4), pp. 846-856

274. Toropov A.A., Toropova A.P., Benfenati E. Erratum: QSAR Modelling for Mutagenic Potency of Heteroaromatic Amines by Optimal SMILES-based Descriptors. (Chemical Biology and Drug Design (2009) 73 (301-312)). (2009) Chemical Biology and Drug Design, 73 (4), p. 482.
275. Eduardo A. Castro, Alla P. Toropova, Andrey A. Toropov and Runet Z. Akhmerov. SMILES-Based QSPR Models of Ionic Lattice Energies. International Journal of Chemical Modeling (Int. J. Chem. Mod) 2 (2009).
276. Toropov A.A., Toropova A.P., Benfenati E. QSAR modelling for mutagenic potency of heteroaromatic amines by optimal SMILES-based descriptors. (2009) Chemical Biology and Drug Design, 73 (3), pp. 301-312.
277. A. A.Toropov, A. P. Toropova, E. Benfenati, A. Manganaro, QSPR modelling of enthalpies of formation for organometallic compounds by SMART-based optimal descriptors. J. Comput. Chem. 30(2009) 2576-2582.
278. E. A. Castro, A. A. Toropov, A. P. Toropova and R. Z. Akhmerov, Optimal descriptors based on extended connectivity and codes of cyles: QSPR of hydrocarbon normal boiling points. Kragujevac J. Sci. 31 (2009) 33-43.

**2008:**

279. Toropov A.A., Toropova A.P., Benfenati E. QSPR modeling for enthalpies of formation of organometallic compounds by means of SMILES-based optimal descriptors. (2008) Chemical Physics Letters, 461 (4-6), pp. 343-347.
280. Toropov A.A., Toropova A.P., Raska Jr. I. QSPR modeling of octanol/water partition coefficient for vitamins by optimal descriptors calculated with SMILES. (2008) European Journal of Medicinal Chemistry, 43 (4), pp. 714-740.
281. A.P. Toropova, A.A. Toropov and I. Gutman, QSPR modelling of water solubility of minerals by optimal descriptors calculated with smiles. Kragujevac J. Sci. 30 (2008) 65-72.

**2006:**

282. Toropova A.P., Toropov A.A., Maksudov S.Kh. QSPR modeling mineral crystal lattice energy by optimal descriptors of the graph of atomic orbitals. (2006) Chemical Physics Letters, 428 (1-3), pp. 183-186.
283. E. A. Castro, A. A. Toropov, A. P. Toropova , R. Z. Akhmerov, QSPR Modeling of the Mineral Crystal Lattice Energy by Optimization of Correlation Weights of Vertex and Vertex Degree in Graph of Atomic Orbitals: Linear and Non-Linear Modes. World Journal of Chemistry 1 (2006) 1-4.

**2005:**

284. Toropov A.A., Toropova A.P., Gutman I. Comparison of QSPR models based on hydrogen-filled graphs and on graphs of atomic orbitals. Croatica Chemica Acta, (2005) 78 (4), pp. 503-509.
285. Gutman I., Toropov A.A., Toropova A.P. The graph of atomic orbitals and its basic properties. 1. Wiener index (2005) Match, 53 (1), pp. 215-224.
286. Gutman I., Furtula B., Toropov A.A., Toropova A.P. The graph of atomic orbitals and its basic properties. 2. Zagreb indices (2005) Match, 53 (1), pp. 225-230.
287. Toropov A.A., Toropova A.P., Mukhamedzhanova, D.V., Gutman, I. Simplified molecular input line entry system (SMILES) as an alternative for constructing quantitative structure-property relationships (QSPR). (2005) Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry, 44 (8), pp. 1545-1552.

288. Castro E.A., Toropova A.P., Toropov A.A., Mukhamedjanova D.V. QSPR modeling of Gibbs free energy of organic compounds by weighting of nearest neighboring codes. (2005) Structural Chemistry, 16 (3), pp. 305-324.

**2004:**

289. Toropov A., Toropova A. Nearest neighboring code and hydrogen bond index in labeled hydrogen-filled graph and graph of atomic orbitals: Application to model of normal boiling points of haloalkanes. (2004) Journal of Molecular Structure: THEOCHEM, 711 (1-3), pp. 173-183.
290. Toropov A.A., Toropova A.P., Nesterova A.I., Nabiev O.M. QSPR modeling of complex stability by correlation weighing of the topological and chemical invariants of molecular graphs. (2004) Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 30 (9), 611-617.
291. Toropov A.A., Toropova A.P., Nesterova A.I., Nabiev O.M. Prediction of alkane enthalpies by means of correlation weighting of Morgan extended connectivity in molecular graphs. (2004) Chemical Physics Letters, 384 (4-6), pp. 357-363.
292. Toropov A.A., Toropova A.P., Nesterova A.I., Nabiev O.M. QSPR modeling of complex stability by correlation weighing of the topological and chemical invariants of molecular graphs. (2004) Russian Journal of Coordination Chemistry/ Koordinatsionnaya Khimiya, 30 (9), pp. 649-655.

**2003:**

293. Toropov A.A., Toropova A.P., Nesterov I.V., Nabiev O.M. Comparison of QSAR models of anti-HIV-1 potencies based on labeled hydrogen filled graph and graph of atomic orbitals. (2003) Journal of Molecular Structure: THEOCHEM, 640, pp. 175-181.
294. Toropov A.A., Toropova A.P. QSPR modeling of alkanes properties based on graph of atomic orbitals. (2003) Journal of Molecular Structure: THEOCHEM, 637, pp. 1-10.
295. Castro E.A., Toropova A.P., Toropov A.A., Mukhamedjanova D.V. QSPR modeling of Gibbs free energy of chemical transformations of oil shale components during thermal treatment. (2003) Anales des la Asociacion Quimica Argentina, 91 (4-6), pp. 85-90.

**2002:**

296. Toropov A.A., Toropova A.P. QSPR modeling of complex stability by optimization of correlation weights of the hydrogen bond index and the local graph invariants. (2002) Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 28 (12), pp. 877-880.
297. Toropov A.A., Toropova A.P. QSPR modeling of complex stability by optimization of correlation weights of the hydrogen bond index and the local graph invariants. (2002) Russian Journal of Coordination Chemistry/ Koordinatsionnaya Khimiya, 28 (12), pp. 938-943.
298. Toropov A.A., Toropova A.P. Modeling of acyclic carbonyl compounds normal boiling points by correlation weighting of nearest neighboring codes. (2002) Journal of Molecular Structure: THEOCHEM, 581, pp. 11-15.
299. Toropov A.A., Toropova A.P. QSAR modeling of toxicity on optimization of correlation weights of Morgan extended connectivity. (2002) Journal of Molecular Structure: THEOCHEM, 578, pp. 129-134.

**2001:**

300. Toropov A.A., Toropova A.P. QSPR modeling of stability of complexes of adenosine phosphate derivatives with metals absent from the complexes of the teaching access. (2001) Russian Journal of Coordination Chemistry/ Koordinatsionnaya Khimiya, 27 (8), pp. 612-616.

301. Toropov A.A., Toropova A.P. QSPR modeling of stability of complexes of adenosine phosphate derivatives with metals absent from the complexes of the teaching access. (2001) Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 27 (8), pp. 574-578.
302. Toropova A.P., Toropov A.A. Using correlation eight optimization of the local invariants of graphs for QSPR simulation of crystal lattice energy. (2001) Journal of Structural Chemistry, 42 (6), pp. 1033-1035.
303. Toropov A.A., Toropova A.P. Modeling of lipophilicity by means of correlation weighting of local graph invariants. (2001) Journal of Molecular Structure: THEOCHEM, 538, pp. 197-199.
304. Toropov A.A., Toropova A.P. Prediction of heteroaromatic amine mutagenicity by means of correlation weighting of atomic orbital graphs of local invariants. (2001) Journal of Molecular Structure: THEOCHEM, 538, pp. 287-293.

**2000:**

305. Toropov A.A., Toropova A.P. QSPR modeling of the formation constants for complexes using atomic orbital graphs. (2000) Russian Journal of Coordination Chemistry/ Koordinatsionnaya Khimiya, 26 (6), pp. 423-430.
306. Toropov A.A., Toropova A.P. QSPR modeling of the stability constants of biometal complexes with phosphate derivatives of adenosine. (2000) Russian Journal of Coordination Chemistry/ Koordinatsionnaya Khimiya, 26 (11), pp. 842-847.
307. Toropova A.P., Toropov A.A., Ishankhodzhaeva M.M., Parpiev N.A. QSPR Modeling of Stability Constants of Coordination Compounds by Optimization of Correlation Weights of Local Graph Invariants. (2000) Russian Journal of Inorganic Chemistry, 45 (7), pp. 1057-1059.
308. Toropov A.A., Toropova A.P. QSPR modeling of the stability constants of biometal complexes with phosphate derivatives of adenosine. (2000) Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 26 (11), pp. 792-797.
309. Toropov A.A., Toropova A.P. QSPR modeling of the formation constants for complexes using atomic orbital graphs. (2000) Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 26 (6), pp. 398-405.

**1999:**

310. Toropov A.A., Toropova A.P., Voropaeva N.L., Ruban J.N., Rashidova S.Sh. Two concepts of weighing molecular graph local invariants in qspr modeling of the enthalpies of complexes: sampling of increments and optimization of correlation weights. (1999) Russian Journal of Coordination Chemistry/ Koordinatsionnaya Khimiya, 25 (9), pp. 664-669.
311. Toropov A.A., Toropova A.P., Voropaeva N.L., Ruban I.N., Rashidova S.Sh. Testing the atomic orbital graph as a basis for QSPR modeling of the boiling points of haloalkanes. (1999) Journal of Structural Chemistry, 40 (6), pp. 950-958.
312. Toropov A.A., Toropova A.P., Voropaeva N.L., Ruban I.N., Rashidova S.Sh. Two concepts of weighing molecular graph local invariants in QSPR modeling of the enthalpies of complexes: Sampling of increments and optimization of correlation weights. (1999) Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 25 (9), pp. 618-623.
313. Toropov A.A., Toropova A.P., Voropaeva N.L., Ruban I.N., Rashidova S.Sh. Using the maximal topological distance matrix for QSPR modeling of the boiling points of cyclic hydrocarbons. (1999) Journal of Structural Chemistry, 40 (1), pp. 169-172.

**1998:**

314. Toropov A.A., Toropova A.P. Optimization of correlation weights of the local graph invariants: Use of the enthalpies of formation of complex compounds for the QSPR modelling. (1998) Russian Journal of Coordination Chemistry/ Koordinatsionnaya Khimiya, 24 (2), pp. 89-93.
315. Toropov A.A., Toropova A.P., Voropaeva N.L., Ruban I.N., Rashidova S. Sh., Generalized zero-order molecular connectivity index: enthalpies of crystalline aquo and ammino complexes in QSPR modelling. (1998) Russian Journal of Coordination Chemistry/ Koordinatsionnaya Khimiya, 24 (8), pp. 563-567.
316. Toropov A.A., Toropova A.P., Voropaeva N.L., Ruban I.N., Rashidova S.Sh. Generalized zero-order molecular connectivity index: Enthalpies of crystalline aquo and ammino complexes in QSPR modelling. (1998) Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 24 (8), pp. 525-529.
317. Toropov A., Toropova A., Ismailov T., Bonchev D. 3D weighting of molecular descriptors for QSPR/QSAR by the method of ideal symmetry (MIS). 1. Application to boiling points of alkanes. (1998) Journal of Molecular Structure: THEOCHEM, 424 (3), pp. 237-247.
318. Toropov A.A., Toropova, A.P. Optimization of correlation weights of the local graph invariants: Use of the enthalpies of formation of complex compounds for the QSPR modelling. (1998) Russian Journal of Coordination Chemistry/ Koordinatsionnaya Khimiya, 24 (2), pp. 81-85.

**1997:**

319. Toropov A.A., Toropova A.P. Method of Ideal Symmetry in Four-Dimensional Space: Implementation in the QSPR Studies on the Thermochemistry of Complex Compounds. (1997) Russian Journal of Coordination Chemistry/ Koordinatsionnaya Khimiya, 23 (10), pp. 789-795.
320. Toropov A.A., Toropova A.P., Ismailov, T.T., Voropaeva, N.L., Ruban, I.N. Extended molecular connectivity: Prediction of boiling points of alkanes. (1997) Journal of Structural Chemistry, 38 (6), pp. 965-969.
321. Toropov A.A., Toropova A.P. Method of ideal symmetry in four-dimensional space: Implementation in the QSPR studies on the thermochemistry of complex compounds. (1997) Russian Journal of Coordination Chemistry/ Koordinatsionnaya Khimiya, 23 (10), pp. 741-747.
322. Toropov A.A., Toropova A.P., Ismailov, T.T., Voropaeva, N.L., Ruban, I.N. Correlations of indices calculated from the matrix of maximal topological distances with boiling points of alkylbenzenes. (1997) Journal of Structural Chemistry, 38 (1), pp. 135-139.

**1996:**

323. Toropov A.A., Toropova A.P., Voropaeva N.L., Ruban J.N., Rashidova S.Sh. Approval of the random mutual orientation statistics index as a basis in search for the structure-property relationship in coordination compounds. (1996) Russian Journal of Coordination Chemistry/ Koordinatsionnaya Khimiya, 22 (7-8), pp. 613-615.
324. Toropov A.A., Toropova A.P., Ismailov T.T., Voropaeva N.L., Ruban I.N., Rashidova S.Sh. The use of deformation indices of the ideal symmetry model in calculations of the thermodynamic properties of organic compounds. (1996) Zhurnal Fizicheskoi Khimii, 70 (7), pp. 1165-1169.
325. Toropova A.P., Toropov A.A., Ishankhodzhaeva M.M., Parpiev N.A. structural analysis of the copper (II) and nickel (II) complexes with nitromethine ligands by the method of ideal symmetry. (1996) Russian Journal of Coordination Chemistry/ Koordinatsionnaya Khimiya, 22 (7-8), pp. 561-564.
326. Toropov A.A., Toropova A.P., Voropaeva N.L., Ruban I.N., Rashidova S.Sh. Approval of the random-mutual-orientation statistics index as a basis for searching for "structure-property" relationships in coordination compounds.(1996) Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 22 (8), pp. 578-580.

327. Toropov A.A., Toropova A.P., Ismailov T.T., Voropaeva N.L., Ruban I.N., Rashidova S.Sh. The use of deformation indices of the ideal symmetry model in calculations of the thermodynamic properties of organic compounds. (1996) Russian Journal of Physical Chemistry A, 70 (7), pp. 1081-1084.
328. Toropova A.P., Toropov A.A., Ishankhodzhaeva M.M., Parpiev N.A. Structural analysis of copper(II) and nickel(II) complexes with azomethine ligands by the method of ideal symmetry. (1996) Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 22 (7), pp. 527-530.

## Conferences and workshops

**SCARLET – Istituto di Ricerche Farmacologiche Mario Negri– April 2-4, 2008**
**1**.A.A. Toropov, A.P. Toropova, E. Benfenati
QSAR modeling of carcinogenicity and mutagenic potency by optimal SMILES-based descriptors **2.** E. Benfenati, A. Chana, A.A. Toropov, A.P. Toropova
QSAR modeling of carcinogenicity based on local attributes of SMILES and special codes of cycles 1st SETAC Europe Special Science Symposium 23-24 October 2008, Brussels
**3.** A. Chana, A.A. Toropov, A.P. Toropova, E. Benfenati, X.-K. Hu, H.-M. Hwang, B.F. Rasulev, T. Puzyn, J. Leszczynski
QSAR modelling of biological activity by descriptors calculated with simplified molecular input line entry system (SMILES)

**SETAC – Goteborg (Sweden) – May 2009**
1. A.A. Toropov, A.P. Toropova and E. Benfenati
QSAR modelling of mutagenicity: the applicability domain definition and the estimation of predictive ability
2. A.A. Toropov, A.P. Toropova, X.-K. Hu, H.-M. Hwang, B.F. Rasulev, T. Puzyn, E. Benfenati, D. Leszczynska, and J. Leszczynski
QSAR model of toxicity towards *E.Coli* bacteria for nanosized oxides by SMILES-based optimal descriptors

**VII World Congress on Alternatives & Animal Use in the Life Sciences – Italy, Rome, September, 2009**
A.A. Toropov, A.P. Toropova, E. Benfenati
Additive smiles-based carcinogenicity models: a new approach to increase robustness and prediction

**Orchestra March 2011, Milan, Italy**
1. Alla. P. Toropova, Andrey A. Toropov, Emilio Benfenati, Giuseppina Gini, Danuta Leszczynska, Jerzy Leszczynski QSAR modeling of toxicity of binary mixtures by CORAL software
2. Andrey A. Toropov, Alla. P. Toropova, Emilio Benfenati, Giuseppina Gini, Danuta Leszczynska, Jerzy Leszczynski QSAR modeling of cytotoxicity of nanoparticles

**SETAC May 2011, Milan, Italy**
1. Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, Giuseppina Gini
SMILES-based QSPR model for Bioconcentration Factor
2. Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, Giuseppina Gini
QSAR for toxicity of aromatic aldehydes to Tetrahymena pyriformis using correlation weights of physicochemical situations
3. Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, Giuseppina Gini
QSAR models for toxicity of organic substances to Daphnia magna built up by using the CORAL freeware

**QSAR 2014, June 16-20, 2014, Milan Italy**
1. F. Pizzo, D. Gadaleta, A. Lombardo, A. A. Toropov, A. P.Toropova, S. E. Escher, O. Nicolotti, A. Carotti, E. Benfenati Different Approaches for Modeling Repeated Dose Toxicity, Lecture
2. Alla P. Toropova, Andrey A. Toropov, Aleksandar M. Veselinović, Jovana B. Veselinović, Emilio Benfenati, Orazio Nicolotti, Angelo Carotti, Danuta Leszczynska, Jerzy Leszczynski Optimal descriptor as a translator of eclectic data into models for mutagencity of fullerene in different conditions, Poster
3.Alla P. Toropova, Andrey A. Toropov, Emilio Benfenati
Quasi-QSPR/QSAR: reasons, tasks, results, Poster
4. V. H. Masand, A. P. Toropova, A. A. Toropov, D. T. Mahajan
QSAR Modeling of Anxiolytic Activity Taking into Account the Presence of Keto-Enol Tautomerism, Poster
5. V. H. Masand, A. A. Toropov, A. P. Toropova, D. T. Mahajan
The Monte Carlo Method as a Tool to Predict Anti-Malarial Activity of 4-Aminoquinolines, Poster

**12th International Conference on Nanosciences (NN15). Thessaloniki, Greece, 7 - 11 July 2015**
Manganelli, S., Leone, C., Toropov, A.A., Toropova, A.P., Benfenati, E. (2015): QSAR model for cytotoxicity of silica nanoparticles on human embryonic kidney cells. (poster presentation).

**CompNanoTox2015. Malaga, Spain, 4-6 November 2015**
Toropova, A.P., Toropova, A.A., Benfenati, E. (2015): Modelling nanomaterials with CORAL. (poster presentation).

**The SETAC Europe 29th Annual Meeting, held on 26-30 May 2019 in Helsinki, Finland**
E. Carnesecchi, A.A. Toropov, A.A. Toropova, N. Kramer, C. Svendsen, J. Dorne, E. Benfenati.
**TU317**: CORAL: innovative open source QSAR model for predicting acute contact toxicity of binary mixtures of plant protection products in honeybee (A. mellifera). (poster presentation).

**Nanosafety workshop - From Molecules to Public Health (November 11-12, 2021, Portugal, Braga).**
Andrey Toropov, Alla Toropova. Cheminformatics and in silico tools: What is Quasi-SMILES? How to use for nano-QSPR/QSAR?

**28th Annual Meeting of the Slovenian Chemical Society (September 21 – 23, 2022, Portorose, Slovenia).**
Natalja Fjodorova, Marjana Novič, Katja Venko, Bakhtiyor Rasulev, Melek Türker Saçan, Gulcin Tugcu, Safiye Sağ Erdem, Elifcan Çalışkan, Alla P. Toropova, Andrey A. Toropov.
Investigation of aquatic toxicity of fullerene derivatives using cheminformatics approach.

**SB05.03.05, April 11, 2023-MRS Spring Meeting & Exhibit in San Francisco.**
B. Rasulev, M. Zamani, S. Szwiec, G. Casanola-Martin, N. Fjodorova, M. Novič, K. Venko, M. Türker, G. Tugcu, S. Erdem, A. Toropova, A. Toropov.
Assessing Toxicity of Fullerene Nanostructures Using Human Proteins by Combined Computational Chemistry and Cheminformatics Approach.
https://www.mrs.org/meetings-events/spring-meetings-exhibits/2023-mrs-spring-meeting/call-for-papers/presentations/detail/2023_mrs_spring_meeting/3838685-202304110845

**CORAL Freeware**
A.A. Toropov, A.P. Toropova, E. Benfenati CORAL freeware (CORrelations And Logic) is available at http://www.insilico.eu/coral
® Istituto di Ricerche Farmacologiche Mario Negri - September, 2009