CURRICULUM VITAE

Surname, firstname, patronymic	**Dr. Toropova Alla P. (Toropova Alla Petrovna)**
Brief service record	1986 - 1991 – Lecturer in Industry College, Uzbekistan 1991 - 1994 – PhD student in Tashkent State University, Uzbekistan 1994 – 1998 – scientific collaborator at Institute of Geology & geophysics of Acad. Sci. Rep. Uzbekistan 1998 - 2007 senior scientific researcher at Institute of Geology & geophysics of Acad. Sci. Rep. Uzbekistan 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. 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". https://www.imrpress.com/journal/FBL/special_issues/1396741473864962049 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". https://www.mdpi.com/journal/molecules/special_issues/QSAR_QSPR_II 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". https://www.mdpi.com/journal/chemistry/special_issues/QSAR_QSPR_Applications 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. 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. 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 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. ***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 ***Member of Editorial Review Board*** of the Journal of Nanotoxicology and Nanomedicine(JNN) http://www.igi-global.com/journal/journal-nanotoxicology-nanomedicine-jnn/126553 ***Member of the Editorial Board*** of the journal " Molecules" https://www.mdpi.com/journal/molecules/editors ***Referee in*** 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

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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, 12th 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 2020
Citations	7659	3829
h-index	45	31
i10-index	216	131

Characterization of Dr. Toropova A.P. by SCOPUS database
http://www.scopus.com/authid/detail.url?authorId=6701335146
h-Index =40 (i.e. there are 40 articles which are cited 40 or more times)

Year	The number of published articles and chapters	The total number of citations up to now
2025	5+0 (in press)	98
2024	9	512
2023	34	737
2022	19	542
2021	20	606

The total number of citations (SCOPUS) is 6361(March 11, 2025)

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

2025:

1. Iovine, N.; Toropova, A.P.; Toropov, A.A.; Roncaglioni, A.; Benfenati, E. Simulation of the Long-Term Toxicity towards Bobwhite Quail (Colinus virginianus) by the Monte Carlo method. J. Xenobiot. 2025, 15, 3. https://doi.org/10.3390/jox15010003
2. Toropova, A.P.; Toropov, A.A.; Roncaglioni, A.; Benfenati, E. In Silico Simulation of Daphnia magna immobilization exposed to mixtures of TiO_2 nanoparticles with inorganic compounds. J. Compos. Sci. 2025, 9, 16. https://doi.org/10.3390/jcs9010016
3. A. P. Toropova, A. A. Toropov, A. Roncaglioni, E. Benfenati, Monte Carlo simulation of aromatic molecules adsorption on multi-walled carbon nanotube surfaces using coefficient of conformism of a correlative prediction (CCCP). C-Journal of Carbon Research, 2025, 11, 7. https://doi.org/10.3390/c11010007
4. Andrey A. Toropov, Alla P. Toropova, Valentin O. Kudyshkin, Danuta Leszczynska, Jerzy Leszczynski, Application of monomer structures and fragments of local symmetry for simulation of glass transition temperatures of polymers. SAR and QSAR in Environmental Research, 2025, 36(1), 29–37. DOI: 10.1080/1062936X.2025.2453868
5. Aleksandar M. Veselinović, Alla P. Toropova, Andrey A. Toropov, Alessandra Roncaglioni, Emilio Benfenati, Las Vegas algorithm in the prediction of intrinsic solubility of drug-like compounds, Journal of Molecular Graphics and Modelling, 137, 2025,109004. https://doi.org/10.1016/j.jmgm.2025.109004

2024:

6. 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
7. Toropova, A.P.; Toropov, A.A.; Roncaglioni, A.; Benfenati, E. Quantitative Structure–Activity Relationship Models for the Angiotensin-Converting Enzyme Inhibitory Activities of Short-Chain Peptides of Goat Milk Using Quasi-SMILES. Macromol 2024, 4, 387-400. https://doi.org/10.3390/macromol4020022
8. E. Benfenati, A. Roncaglioni, N. Iovine, M. Marzo, A. Toropov, A. Toropova, A. Ciacci, M. Lettieri, L. Sartori, C. Yang, T. Magdziarz, B. Hobocienski, A. Mostrag, Istituto di Ricerche Farmacologiche Mario Negri, Molecular Networks and S-IN Soluzioni Informatiche, 2023. Maintenance, update and further development of EFSA's Chemical Hazards Database: OpenFoodTox 2.0. EFSA supporting publication 2024: 21(1): EN-8590. 40 pp. doi:10.2903/sp.efsa.2024.EN-8590
9. 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 2024, 47, 3, 306–313. https://doi.org/10.1080/01480545.2023.2174986
10. Iovine, N.; Toropova, A.P.; Toropov, A.A.; Roncaglioni, A.; Benfenati, E. Models for the No-Observed-Effect Concentration (NOEC) and Maximal Half-Effective Concentration (EC50). Toxics 2024, 12, 425. https://doi.org/10.3390/toxics12060425
11. 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. Journal of Mathematical Chemistry (2024) 62: 2373–2387. https://doi.org/10.1007/s10910-023-01517-0

12. 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, 2024, 34(7), 737–742. https://doi.org/10.1080/15376516.2024.2332617
13. Alla P. Toropova, Andrey A. Toropov, Natalia Sizochenko, Using the vector of the ideality of correlation to simulate the zeta potential of nanoparticles under different experimental conditions, represented by quasi-SMILES. Structural Chemistry, (2024) 35:1925–1935.
DOI: 10.1007/s11224-024-02357-7
14. F. Bazzi-Allahri, F. Shiri, S. Ahmadi, A.P. Toropova, A.A. Toropov, SMILES-based QSAR virtual screening to identify potential therapeutics for COVID-19 by targeting 3CLpro and RdRp viral proteins. BMC Chemistry, (2024) 18:191. https://doi.org/10.1186/s13065-024-01302-3

2023:

15. 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
16. 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
17. 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
18. 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
19. 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
20. 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
21. 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
22. 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
23. 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
24. 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
25. 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
26. 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
27. 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
28. 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
29. 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
30. 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
31. 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
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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

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