

CURRICULUM VITAE

Surname, firstname, patronymic

Dr. Toropov Andrey A. (Toropov Andrey Andreevich)

Brief service record

1986 - 1987 – engineer in the Institute of Chemistry Acad. Sci. UzSSR.
1987 - 1991 – junior researcher of the Polymer Chemistry and Physics Academy of Science Rep. Uzbekistan
1991-1993 - Tashkent secondary school 225, teacher of computer sciences, Uzbekistan
1994-2002 research worker of the Institute of Polymer Chemistry and Physics, Acad. Sci. Rep. Uzbekistan
2002 – 2004 senior scientific researcher at the ‘Algorithm – Engineering’ institute of Acad. Sci. Rep. Uzbekistan
2004 - 2005 senior scientific researcher at the Institute of Geology & Geophysics of the Academy Sci. Rep. Uzbekistan
2005 – joint QSAR study in Istituto di Ricerche Farmacologiche Mario Negri, Milano, Italy
2006 – 2007 joint QSPR/QSAR analysis for nanomaterials in Computational Center for Molecular Structure and Interactions, Jackson State University, Jackson, MS, USA
2007-2009 Marie Curie fellowships at Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy
2009-up to present invited scientist at Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milano, Italy

Scientific interest

Quantitative Structure –Property/Activity Relationships (QSPR/QSAR); analysis of nano materials

Scientific degree

Ph.D. in mathematics and physics (1998)

Membership in Editorial Board of scientific journals

2025, Guest Editor of an issue of Discover Nano; Special issue: "QSPR/QSAR for Nano Phenomena: Recent Developments, Applications, and Ideas". <https://link.springer.com/collections/fbfaijfhje>
2024, Guest Editor of an issue of Toxics (impact factor =4.1); Special issue: "Advances in Computational Toxicology and Their Exposure". This special issue belongs to the section "Novel Methods in Toxicology Research". https://www.mdpi.com/journal/toxics/special_issues/Q5K6T2BTG0
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) (IF=3.295); Special issue: "From Chemoinformatics to Nanoinformatics: New tools for Drug Discovery and Nanoparticles Design in Medicinal Chemistry"; Vol. 15, No. 18
2015, Member of Scientific Committee of "Mol2Net, International Conference on Multidisciplinary Sciences- 2015", 1, pages 1-4, doi: 10.13140/RG.2.1.3123.3122 ; <http://sciforum.net/conference/mol2net-1>
2004, Guest editor on Special issue "Recent Advances in Flexible Molecular Descriptors In QSAR/QSPR Theory" (European Journal Molecules)

Member of the Advisory Editorial Board of the Journal of Argentine Chemical Society <http://www.scielo.org.ar/revistas/jacs/cedboard.htm>

Member of the Advisory Editorial Board of the section "Molecular Design and Informatics" in the journal "Combinatorial Chemistry & High Throughput Screening"
<https://benthamscience.com/journals/combinatorial-chemistry-and-high-throughput-screening/editorial-board/>

Member of the Advisory Editorial Board of the journal "Current Drug Discovery Technologies" <https://benthamscience.com/journals/current-drug-discovery-technologies/editorial-board/>

Member of the Editorial Board member of the journal "Toxics" <https://www.mdpi.com/journal/toxics/editors>

Member of the Editorial Board member of the journal "Mini-Reviews in Medicinal Chemistry" (MRMC) <https://benthamscience.com/journals/mini-reviews-in-medicinal-chemistry/editorial-board/>

Member of the 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 Review Board of the International Journal of Quantitative Structure-Property Relationships (IJQSPR) <http://www.igi-global.com/journal/international-journal-quantitative-structure-property/126552>

Referee in

ARKIVOC (USA), <http://www.arkat-usa.org>
Chemosphere
Computers in Biology and Medicine
Bioorganic and Medicinal Chemistry
Bioorganic and Medicinal Chemistry Letters
Acta Chemica Slovenia
Central European Journal of Chemistry
Chemometrics and Intelligent Laboratory Systems
European polymer
International Journal of Molecular Sciences
Environmental Analytical Chemistry
Chemical Biology and Drug Design
Journal of Molecular Graphics and Modeling
Journal of Physical Chemistry (ACS)
Analytica Chimica Acta
Electrochimica Acta
Journal of Computational Chemistry
Molecular Diversity
Chemical Research in Toxicology
Water Sciences and Technology
Molecules

Abroad trips

2002. Lion, France
2004. Milan, Italy
2005-2006. Milan, Italy
2006 Prague, Check Republic
2006-2007 Jackson, MS, USA
2007- up to present Milan, Italy

Address

20156, Via Mario Negri, 2, Milan, Italy

Email

andrey.toropov@marionegri.it
aatoropov@yahoo.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](#): 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
[February 26, 2014](#), XXXIV ELBA NANOFORUM. Nanomedicine Workshop, Laboratories of Biophysics and Nanobiotechnology, DIMES, Genova University, Italy.
[June 4-6, 2013](#), Harmonization 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
[17-22 March 2013](#), Fourth Nanosafety Annual School: Understanding Human Health Effects and Environmental Impacts of Engineered Nanomaterials, Venice, Italy.
[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
[May, 2009](#), SETAC, Goteborg, Sweden
[March, 2008](#), SCARLET–Istituto di Ricerche Farmacologiche Mario Negri, Milan, Italy
[October, 2007](#), 15th Conference on Current Trends in Computational Chemistry – Jackson State University, Jackson, USA, MI,

Participation in International scientific grants

CHEMPREDICT (n. MIF1-CT-2006-039036)
 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)
 LIFE-CONCERT contract (LIFE17 GIE/IT/000461)

Development of the **CORAL Freeware** (**COR**relations **And** **L**ogic),
<http://www.insilico.eu/coral>, CHEMPREDICT (039036).

Characterization of Dr. Toropov A.A. by Google Scholar Citations

<https://scholar.google.co.uk/citations?user=TfckQOIAAAAJ&hl=en>

Citation indices	All	Since 2021
Citations	11524	4238
h-index	52	28
i10-index	291	142

Characterization of Dr. Toropov A.A. by SCOPUS database

<http://www.scopus.com/authid/detail.url?authorId=7102208151>

h-Index=45 (i.e., there are 45 articles that are cited 45 or more times)

Year	The number of published articles and chapters	The total number of citations up to now
2026	6 +2 (in press)	187
2025	19	597
2024	10	564

2023	34	834
2022	20	629

The total number of citations (SCOPUS) is 9282 (May 22, 2026)

PUBLICATION LIST OF ANDREY A. TOROPOV

Chapters in Books and other publications:

- A.P. Toropova, A.A. Toropov, E. Benfenati, **Chapter 9**. Simulation of physicochemical and biochemical behavior of nanoparticles under various experimental conditions. **In:** Roy, K., Banerjee, A. (eds) *Cheminformatic Modeling and Data Gap Filling for a Green and Sustainable Environment*, 2026, 1st Edition - May 1, 2026. Elsevier. eBook ISBN: 9780443364754. <https://shop.elsevier.com/books/cheminformatic-modeling-and-data-gap-filling-for-a-green-and-sustainable-environment/roy/978-0-443-36474-7>
- Toropov, A.A., Toropova, A.P., Roncaglioni, A., Benfenati, E. **Chapter 19**. Quasi-SMILES as a tool for simulation of endpoints related to nanomaterials. *In: Alfaro-Moreno, E., Murphy, F. (eds) Nanosafety*. 2025, pp 531–557. Springer, Cham. https://doi.org/10.1007/978-3-031-93871-9_19
- N. Fjodorova, M. Novič, K. Venko, B. Rasulev, M. Türker Saçan, G. Tugcu, S. Sağ Erdem, A.P. Toropova, A.A. Toropov, **Chapter 6**. Applications of Predictive Modeling for Fullerenes. *In: Roy, K., Banerjee, A. (eds) Materials Informatics II. Challenges and Advances in Computational Chemistry and Physics*, 2025, vol. 40, pp. 133–151. Springer, Cham. https://doi.org/10.1007/978-3-031-78728-7_6
- **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
- Nesměrák, K., Toropov, A.A. **Chapter 6**. QSPR Models for Prediction of Redox Potentials Using 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 139-166. Springer, Cham. https://doi.org/10.1007/978-3-031-28401-4_6
- 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 Al₂O₃ 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. Bacao, 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., Alzheimer's disease: SMILES to preserve wisdom. **2015.** *Available on the Atlas of Science website:* <http://atlasofscience.org/alzheimers-disease-smiles-to/>
- 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. Bacao, 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>
- Georgia Melagraki, Antreas Afantitis, Andrey A. Toropov, Haralambos Sarimveis, Olga Igglessi – Markopoulou,
Chapter 4. QSAR models constructed by optimal descriptors and by multiple regression analysis for the prediction of carbonic anhydrase II inhibitory activity of substituted

aromatic sulphonamides. **In Book:** *E.A. Castro (Eds.) QSPR-QSAR Studies on Desired Properties for Drug Design*, **2010**, 95-116. ISBN: 978-81-308-0404-0.
http://www.trnres.com/ebook/uploads/castro/T_1310531320Castro%204.pdf

- A.A. Toropov, B.F. Rasulev, D. Leszczynska, and J. Leszczynski, **Chapter 14.** New Approach to QSPR Modeling of Fullerene C60 Solubility in Organic Solvents: An Application of SMILES- Based Optimal Descriptors. **In Book:** *F. Cataldo, and T.Da Ros. (Eds.) Medicinal Chemistry and Pharmacological Potential of Fullerenes and Carbon Nanotubes*, Vol. 1, **2008**, pp. 337-350.
<http://www.springerlink.com/content/978-1-4020-6844-7>

Articles in Impacted (or Peer-reviewed) Journals

2026:

1. Alla P. Toropova, Andrey A. Toropov, Sofia Mescieri, Alessandra Roncaglioni and Emilio Benfenati, Simulation of the impact of pesticides on pollinators under different conditions using correlation weighting of quasi-SMILES components together with the Index of Ideality of Correlation (IIC). *Journal of Xenobiotics*, 2026, 16(1), 10. <https://doi.org/10.3390/jox16010010>
2. Andrey A. Toropov, Alla P. Toropova, Simone Stefano, Alessandra Roncaglioni and Emilio Benfenati, Simulation of polydimethylsiloxane-water partition coefficients for organic compounds using the CORAL software. *Structural Chemistry*, Accepted Mar 15, 2026. <https://doi.org/10.1007/s11224-026-02771-z>
3. Benfenati E., Roncaglioni A., Iovine N., Toropov A., Toropova A., Ciacci A., Sartori L., Valerio M., Hobocienski B., Marusczyk J., Sacher O., Schwab C. H., 2026. Further development and update of EFSA's Chemical Hazards database: OpenFoodTox 3.0. EFSA supporting publication 2026:23(4):EN-10099. 104 pp. doi:10.2903/sp.efsa.2026.EN-10099
4. A.P. Toropova, A.A. Toropov, G. Selvestrel, N. Iovine, A. Roncaglioni & E. Benfenati. QSPR models for water solubility of organic compounds using correlation intensity index and Las Vegas algorithm, SAR and QSAR in Environmental Research, 37(4), 2026, 299-310. DOI: 10.1080/1062936X.2026.2659325
5. Toropova, A.P.; Toropov, A.A.; Raška, I., Jr.; Raškova, M.; Achary, P.G.R. QSAR Models for Sweetness: Can They Shape the Future of Nutritional Safety? *Foods* 2026, 15, 1481. <https://doi.org/10.3390/foods15091481>
6. Toropova, A.P.; Toropov, A.A.; Iovine, N.; Selvestrel, G.; Roncaglioni, A.; Benfenati, E. QSAR Models for Repeated Dose Toxicity in Rats Using the CORAL Software. *Toxics* 2026, 14, 338. <https://doi.org/10.3390/toxics14040338>
7. Andrey A. Toropov, Erika Colombo, Alla P. Toropova, Anna Lombardo, Edoardo Luca Viganò, Alessandra Roncaglioni and Emilio Benfenati, Simulation of chronic aquatic toxicity toward fish using the Las Vegas algorithm and the vector of ideality of correlation. *Environmental Toxicology and Chemistry*, Accepted May 18, 2026.

2025:

8. 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>
9. Toropova, A.P.; Toropov, A.A.; Roncaglioni, A.; Benfenati, E. In Silico Simulation of *Daphnia magna* immobilization exposed to mixtures of TiO₂ nanoparticles with inorganic compounds. *J. Compos. Sci.* 2025, 9, 16. <https://doi.org/10.3390/jcs9010016>
10. 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>

11. 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
12. 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>
13. N. Mousa, H. P. Varbanov, V. Kaipanchery, E. Gabano, M. Ravera, A. A. Toropov, L. Charochkina, F. Menezes, G. Godin, I. V. Tetko. On-line OCHEM multi task model for solubility and lipophilicity prediction of platinum complexes. Journal of Inorganic Biochemistry 269 (2025) 112890. <https://doi.org/10.1016/j.jinorgbio.2025.112890>
14. Shahram Lotfi, Shahin Ahmadi, Alla P. Toropova, Andrey A. Toropov, Monte Carlo approach to study the impact sensitivity of nitro compounds using correlation weights of the fragments of molecular structures. Scientific Reports, (2025) 15:11160. <https://doi.org/10.1038/s41598-025-95129-0>
15. Toropov, A.A.; Toropova, A.P.; Roncaglioni, A.; Benfenati, E. Semi-Correlations for the Simulation of Dermal Toxicity. Toxics 2025, 13, 235. <https://doi.org/10.3390/toxics13040235>
16. Toropova, A.P.; Toropov, A.A.; Roncaglioni, A.; Benfenati, E. Using the Coefficient of Conformism of a Correlative Prediction in simulation of cardiotoxicity. Toxics. 2025; 13(4):309. <https://doi.org/10.3390/toxics13040309>
17. Toropova, A.P.; Toropov, A.A.; Benfenati, E. Monte Carlo simulation of pesticide toxicity for Rainbow Trout (*Oncorhynchus mykiss*) Using New Criteria of Predictive Potential. J. Xenobiot. 2025, 15, 82. <https://doi.org/10.3390/jox15030082>
18. Alla P. Toropova, Andrey A. Toropov, Alessandra Roncaglioni, Emilio Benfenati, In silico models of biological activities of peptides using the coefficient of conformism of a correlative prediction and the Las Vegas algorithm. Macromol 2025, 5(2), 27. <https://doi.org/10.3390/macromol5020027>
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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

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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 mutagenicity 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. Toropov, 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