CURRICULUM VITAE

Surname, firstname, patronymic

Dr. Toropov Andrey A. (Toropov Andrey Andreevich)

Brief service record

1986 - 1987 – engineer in Institute of chemistry Acad. Sci. UzSSR.
1987 - 1991–junior researcher of polymer chemistry and physics Acad. Sci. Rep. Uzbekistan
1991-1993 - Tashkent secondary school 225, teacher of computer sciences, Uzbekistan
1994-2002 research worker of institute of polymer chemistry and physics Acad. Sci. Rep. Uzbekistan
2002 – 2004 senior scientific researcher at 'Algorithm – Engineering' institute of Acad. Sci. Rep. Uzbekistan
2004 - 2005 senior scientific researcher at 'Institute of Geology & geophysics of Acad. 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 in 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

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/eedboard.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
Environmatal Analytical Chemistry
Chemical Biology and Drug Design
Journal of Molecular Graphics and Modeling
Journal of Physical Chemistry (ACS)
Analytica Chemica 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

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, 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
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, 15-th 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 **A**nd **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 2017**
Citations	8228	4176
h-index	45	30
i10-index	232	136

Characterization of Dr. Toropov A.A. by SCOPUS database
http://www.scopus.com/authid/detail.url?authorId=7102208151
h-Index=38 (i.e. there are 38 articles which are cited 38 or more times)

Year	**The number of published articles and chapters**	**The total number of citations up to now**
2022	9+5(in press)	276
2021	20	694
2020	27	821
2019	24	594
2018	24	526

The total number of citations (SCOPUS) 6704 (May 30, 2022)

CiteScore 2021- 27,73

PUBLICATION LIST OF ANDREY A. TOROPOV

Chapters in Books and other publications:

- **Alla P. Toropova and Andrey A. Toropov**, Use of the Monte Carlo Method to Build up QSPR/QSAR Models: Index of Ideality of Correlation and Correlation Intensity Index. ***Chapter 3*** *(pp.111-156),* In Book: Thomas B. Hall (Ed.), Monte Carlo Methods: History and Applications. Series: Mathematics Research Developments. Nova, **2020**. 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**, Prediction of Biochemical Endpoints by the CORAL Software: Prejudices, Paradoxes, and Results. ***Chapter 27*** *(pp. 573-583)*, In Book: Orazio Nicolotti (ed.), Computational Toxicology: Methods and Protocols, Methods in Molecular Biology, vol. 1800, https://doi.org/10.1007/978-1-4939-7899-1_27, © Springer Science+Business Media, LLC, part of Springer Nature **2018**.
- **Andrey A. Toropov and Alla P. Toropova**. Improved Model for Biodegradability of Organic Compounds: The Correlation Contributions of Rings. ***Chapter 8*** *(pp. 147-183)*, In Book: Bidoia E., Montagnolli R. (Eds) Toxicity and Biodegradation Testing. Methods in Pharmacology and Toxicology. Humana Press, New York, NY. **2018**. DOI: 10.1007/978-1-4939-7425-2_8
- **Alla P. Toropova, Andrey A. Toropov, Emilio Benfenati, Robert Rallo, Danuta Leszczynska and Jerzy Leszczynski**: Development of Monte Carlo Approaches in Support of Environmental Research. ***Chapter*** **12** (*pages 453-469*), In Book: Advances in QSAR modeling. ***Volume 24*** of the series Challenges and Advances in Computational Chemistry and Physics. Edited: Roy, K. Springer International Publishing AG, 25 May **2017**
- **Alla P. Toropova, Andrey A. Toropov, Aleksandar M. Veselinović, Jovana B. Veselinović, Danuta Leszczynska, Jerzy Leszczynski**: Quasi-Smiles as a novel tool for Prediction of Nanomaterials' endpoints. ***Chapter 8*** (*pages 191-221*), In Book: Multi-Scale Approaches in Drug Discovery: From Synthetic Methodologies and Biological Assays to In Silico Experiments and Back. Edited: Speck-Planche A. Elsevier Science & Technology Books, **2nd March 2017 -** 238 pagine. ISBN: 0081011296, 9780081011294
- **Alla P. Toropova, P. Ganga Raju Achary, Andrey A. Toropov**: Quasi-SMILES for Nano-QSAR Prediction of Toxic Effect of Al_2O_3 Nanoparticles. ***Chapter 59*** (*pages 1573-1584*), In Book: Pharmaceutical Sciences: Breakthroughs in Research and Practice (2 Volumes) **2017** |Pages: 1584. DOI: 10.4018/978-1-5225-1762-7
- **Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, Orazio Nicolotti, Angelo Carotti, Karel Nesmerak, Aleksandar M. Veselinović, Jovana B. Veselinović, Pablo R. Duchowicz, Daniel Bacelo, Eduardo A. Castro, Bakhtiyor F. Rasulev, Danuta Leszczynska, Jerzy Leszczynski**: QSPR/QSAR Analyses by Means of the CORAL Software: Results, Challenges, Perspectives. ***Chapter 36*** (*pages 929-955*), In Book: Pharmaceutical Sciences: Breakthroughs in Research and Practice (2 Volumes) **2017** |Pages: 1584. 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.:** Development of the latest tools for building up "nano-QSAR": Quantitative features—property/activity relationships (QFPRs/QFARs). ***Chapter 12***, In Book: Practical Aspects of Computational Chemistry IV. J. Leszczynski, M.K. Shukla (Eds.). Springer **2016**. ISBN 78-1-4899-7699-4, p. 353-396. DOI: 10.1007/978-1-4899-7699-4_12 http://rd.springer.com/chapter/10.1007%2F978-1-4899-7699-4_12
- **Toropov A.A.,** Alzheimer's disease: SMILES to preserve wisdom. December 22, **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. November 11, **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**, QSPR/QSAR analyses by means of the CORAL software: results, challenges, perspectives. ***Chapter 15***, in Book: Roy, K. (**2015**). Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment (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** Book: QSPR-QSAR Studies on Desired Properties for Drug Design, **2010**: 95-116 ISBN: 978-81-308-0404-0 Editor: Eduardo A. Castro. ***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. http://www.trnres.com/ebook/uploads/castro/T_1310531320Castro%204.pdf
- **A.A. Toropov, B.F. Rasulev, D. Leszczynska, and J. Leszczynski**. New Approach to QSPR Modeling of Fullerene C60 Solubility in Organic Solvents: An Application of SMILES-Based Optimal Descriptors. ***Chapter 14***, pp. 337-350 in Book: Medicinal Chemistry and Pharmacological Potential of Fullerenes and Carbon Nanotubes, Volume 1, **2008**, Edited by F. Cataldo, and T.Da Ros., http://www.springerlink.com/content/978-1-4020-6844-7

Articles in Impacted (or Peer-reviewed) Journals

2022:

1. 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
2. A.A. Toropov, F. Kjeldsen, A.P. Toropova, Use of quasi-SMILES to build models based on quantitative results from experiments with nanomaterials. Chemosphere, Accepted 21 May, 2022. https://doi.org/10.1016/j.chemosphere.2022.135086
3. Alla P. Toropova and Andrey A. Toropov, Quasi-SMILES as a basis to build up models of endpoints for nanomaterials. Environmental Technology, Accepted May 29, 2022.
4. 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
5. 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
6. 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
7. 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, Available online March 14, 2022. https://doi.org/10.1080/15376516.2022.2053918

8. 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, Accepted Jan 22, 2021. DOI: 10.1080/09593330.2021.1882588
9. K. Nesměrák, A.A. Toropov, I. Yildiz, QSAR based on hybrid optimal descriptors as a tool to predict antibacterial activity against *Staphylococcus aureus*. Front. Biosci. (Landmark Ed), 2022; 27(4): 112. http://doi.org/10.31083/j.fbl2704112
10. 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
11. 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
12. 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
13. 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
14. 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, Accepted May 9, 2022. DOI:10.1080/1062936X.2022.2076736

2021:

15. 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
16. 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
17. 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
18. 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
19. 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.
20. 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

21. 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
22. 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
23. 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
24. 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
25. 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
26. 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
27. 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
28. 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
29. 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
30. 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
31. 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
32. 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
33. 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
34. 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:

35. 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
36. 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.
37. 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.
38. 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.
39. 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.
40. 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.
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Conferences and workshops

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1.A.A. Toropov, A.P. Toropova, E. Benfenati
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3. A. Chana, A.A. Toropov, A.P. Toropova, E. Benfenati, X.-K. Hu, H.-M. Hwang, B.F. Rasulev, T. Puzyn, J. Leszczynski
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1. A.A. Toropov, A.P. Toropova and E. Benfenati
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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
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A.A. Toropov, A.P. Toropova, E. Benfenati
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1. Alla. P. Toropova, Andrey A. Toropov, Emilio Benfenati, Giuseppina Gini
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2. Andrey A. Toropov, Alla. P. Toropova, Emilio Benfenati, Giuseppina Gini,
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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

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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).

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Andrey Toropov, Alla Toropova. Cheminformatics and in silico tools: What is Quasi-SMILES? How to use for nano-QSPR/QSAR?