Curriculum Vitae

Personal information

Emilio Benfenati

Work experience

January 2021 - present

Head of the Department of Environmental Health Sciences, Istituto di Ricerche Farmacologiche “Mario Negri”, Via Mario Negri 2, Milano, Italy

Activities: Coordination and management of the Department and its research projects. The Department is composed of 4 laboratories with about 70 persons in total. The research activities are: risk assessment, in silico models, chemical analysis of contaminants, bioassays, food assessment.

January 1997 – December 2020

Head of the Laboratory of Environmental Chemistry and Toxicology, Istituto di Ricerche Farmacologiche “Mario Negri”, Via Mario Negri 2, Milano, Italy

Activities: Coordination and management of 21 EU funded projects; participation in 31 other EU funded projects, research activities in the fields of toxicity and environmental modelling, computer chemistry, molecular descriptors, QSARs, toxicity prediction, environmental toxicology, environmental management, characterisation and assessment of contaminants, metabolism studies risk assessment; development of QSAR models for aquatic toxicity, terrestrial toxicity, carcinogenicity, mutagenicity, endocrine disruptors; development of integrated models combining different inputs; analysis of environmental and food samples for pollutants such as dioxins, PCB, PAH, pesticides, endocrine disruptors, industrial pollutants; environmental assessment; impact of pollutions into the environment and human health; former member of the commission for pesticide evaluation for Italy; organization of workshops, seminars, and schools on QSAR and modeling; teaching for courses of Regione Lombardia for "Specialists in Pharmacological Research" and "Technicians in Biochemical Research". Coordinator of three projects funded by German UBA. Coordinator of one project funded by the Italian MIUR. Organization of scientific conferences and workshop. He organized many international conferences and workshops, including the SETAC Europe Conference, May 2011 (2350 participants), and QSAR 2014. Organization of training courses on in silico models.

January 1987 - December 1996

Head of the Biomedical Mass Spectrometry Unit, Istituto di Ricerche Farmacologiche “Mario Negri”, Via Eritrea 53, Milano, Italy

Activities: Analysis of pharmaceuticals, organic compounds in mass spectrometry (pesticides, dioxins, PCB, PAH, endocrine disruptors, other pollutants).

November 1984 – December 1996

Senior researcher, Istituto di Ricerche Farmacologiche “Mario Negri”, Via Eritrea 53, Milano, Italy

Activities: Analysis of pharmaceuticals, organic compounds in mass spectrometry (pesticides, dioxins, PCB, PAH, endocrine disruptors, other pollutants).

November 1983 – October 1984

Researcher, Stanford Magnetic Resonance Laboratory, Stanford University School of Medicine, 299 Campus Drive West, Stanford, California, USA

Activities: Analysis of biological samples by NMR and mass spectrometric methods (in collaboration with Berkeley University)

October 1981 – October 1983

Researcher, Istituto di Ricerche Farmacologiche “Mario Negri”, Via Eritrea 53, Milano, Italy

Activities: Analysis of pharmaceuticals and dioxins.

November 1979 – September 1981

Researcher, Istituto di Ricerche Farmacologiche “Mario Negri”, Via Eritrea 53, Milano, Italy

Activities: synthesis of pharmaceuticals

Istituto Biochimico Italiano Giovanni Lorenzini, Via Lorenzini 1, Milano, Italy

Education and training

September 1982 - June 1985

Post-degree specialisation in Pharmacological Research

Istituto di Ricerche Farmacologiche "Mario Negri", Via Eritrea 53, Milano, Italy

Topic: analysis of pharmaceuticals by mass spectrometry

September 1973 – October 1979

Chemistry degree (summa cum laude)

Università degli Studi di Milano, Istituto di Chimica Organica, 21, Via Giacomo Venezian, I-20133, Milan, Italy

Additional information

Publications

Papers in journals:

2023

Audebert M, Assmann A-S, Azqueta A, Babica P, Benfenati E, Bortoli S, Bouwman P, Braeuning A, Burgdorf T, Coumoul X, Debizet K, Dusinska M, Ertych N, Fahrer J, Fetz V, Le Hégarat L, López de Cerain A, Heusinkveld HJ, Hogeveen K, Jacobs MN, Luijten M, Raitano G, Recoules C, Rundén-Pran E, Saleh M, Sovadinová I, Stampar M, Thibol L, Tomkiewicz C, Vettorazzi A, Van de Water B, El Yamani N, Zegura B, Oelgeschläger M

New approach methodologies to facilitate and improve the hazard assessment of non-genotoxic carcinogens—a PARC project

Frontiers in Toxicology, 5, 2023, https://www.frontiersin.org/articles/10.3389/ftox.2023.1220998.

DOI=10.3389/ftox.2023.1220998

Caballero Alfonso AY, Chayawan C, Gadaleta D, Roncaglioni A, Benfenati E.

A KNIME Workflow to Assist the Analogue Identification for Read-Across, Applied to Aromatase Activity.

Molecules. 2023; 28(4):1832. https://doi.org/10.3390/molecules28041832 (IF 4.927, 2022)

Danieli A, Colombo E, Raitano G, Lombardo A, Roncaglioni A, Manganaro A, Sommovigo A, Carnesecchi E, Dorne J-LCM, Benfenati E.

The VEGA Tool to Check the Applicability Domain Gives Greater Confidence in the Prediction of In Silico Models.

International Journal of Molecular Sciences. 2023; 24(12):9894. https://doi.org/10.3390/ijms24129894 (IF 6.208)

Report of the First ONTOX Stakeholder Network Meeting: Digging Under the Surface of ONTOX Together With the Stakeholders.

Altern Lab Anim. 2024 Jan 18:2611929231225730. doi: 10.1177/02611929231225730. Kalian AD, Benfenati E, Osborne OJ, Gott D, Potter C, Dorne J-LCM, Guo M, Hogstrand C.

Exploring Dimensionality Reduction Techniques for Deep Learning Driven QSAR Models of Mutagenicity.

Toxics. 2023; 11(7):572. https://doi.org/10.3390/toxics11070572

Klambauer G, Clevert D-A, Shah I, Benfenati E, Tetko IV

Introduction to the Special Issue: AI meets Toxicology

Chem. Res. Toxicol. 2023. https://doi.org/10.1021/acs.chemrestox.3c00217 (IF 3.973)

Toropov AA, Barnes DA, Toropova AP, Roncaglioni A, Irvine AR, Masereeuw R, Benfenati E.

CORAL Models for Drug-Induced Nephrotoxicity.

Toxics. 2023; 11(4):293. https://doi.org/10.3390/toxics11040293 (IF 4.472)

Toropov AA, Di Nicola MR, Toropova AP, Roncaglioni A, Dorne JLCM, Benfenati E.

Quasi-SMILES: Self-consistent models for toxicity of organic chemicals to tadpoles.

Chemosphere. 2023 Jan;312(Pt 1):137224. doi: 10.1016/j.chemosphere.2022.137224. (IF 8.943, 2022)

Toropov AA, Toropova AP, Roncaglioni A, Benfenati E

The system of self-consistent models for pesticide toxicity to Daphnia magna,

Toxicology Mechanisms and Methods, (2023) DOI: 10.1080/15376516.2023.2197487 (IF 4.019, 2023)

Toropov AA, Toropova AP, Roncaglioni A, Benfenati E

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. 2. (2023). 10.1039/D3VA00012E.

Toropov AA, Toropova AP, Roncaglioni A, Benfenati E

In silico prediction of the mutagenicity of nitroaromatic compounds using correlation weights of fragments of local symmetry

Mutation Research/Genetic Toxicology and Environmental Mutagenesis, Volume 891, 503684 (2023)

https://doi.org/10.1016/j.mrgentox.2023.503684.

Toropova AP, Toropov AA, Roncaglioni A, Benfenati E.

The System of Self-Consistent Models: QSAR Analysis of Drug-Induced Liver Toxicity.

Toxics. 2023; 11(5):419. https://doi.org/10.3390/toxics11050419 (IF 4.472)

Toropova AP, Toropov AA, Roncaglioni A, Benfenati E

Binding organophosphate pesticides to acetylcholinesterase: Risk assessment using the Monte Carlo method

Toxicological & Environmental Chemistry. 2023. DOI: 10.1080/02772248.2023.2181348 (IF 1.39)

Toropova AP, Toropov AA, Roncaglioni A, Benfenati E.

The enhancement scheme for the predictive ability of QSAR: A case of mutagenicity.

Toxicol In Vitro. 2023 Sep;91:105629. doi: 10.1016/j.tiv.2023.105629. (IF 3.2)

Toropova AP, Toropov AA, Roncaglioni A, Benfenati E.

Using the Correlation Intensity Index to Build a Model of Cardiotoxicity of Piperidine Derivatives.

Molecules. 2023; 28(18):6587. https://doi.org/10.3390/molecules28186587

Toropova AP, Toropov AA, Roncaglioni A, Leszczynska D, Leszczynski J

The validation of predictive potential via the system of self-consistent models: the simulation of blood–brain barrier permeation of organic compounds.

J Mol Model 29, 218 (2023). https://doi.org/10.1007/s00894-023-05632-2 (IF 2.172)

Toropova AP, Toropov AA, Roncaglioni A, Leszczynska D, Leszczynski J

CORAL: Model of Ecological Impact of Heavy Metals on Soils via the Study of Modification of Concentration of Biomolecules in Earthworms (Eisenia fetida).

Arch Environ Contam Toxicol 84, 504–515 (2023). https://doi.org/10.1007/s00244-023-01001-5 (IF 3.692)

2022

Benfenati E, Roncaglioni A, Edoardo Carnesecchi, Matilda Mazzucotelli, Marco Marzo, Andrey Toropov, Alla Toropova, Rossella Baldin, Andrea Ciacci, Simona Kovarich, Luca Sartori, Chihae Yang, Tomasz Magdziarz, Bryan Hobocienski, Aleksandra Mostrag

Maintenance, update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0

EFSA Supporting Publications, Vol 19, Issue 12, 2022, 7635E

Biggi G, Giuliani E, Martinelli A, Benfenati E

Patent Toxicity

Research Policy 51 (2022) 104329

Caballero Alfonso AY, Mora Lagares L, Novic M, Benfenati E, Kumar A, Chayawan

Exploration of structural requirements for azole chemicals towards human aromatase CYP19A1 activity: Classification modeling, structure-activity relationships and read-across study,

Toxicology in Vitro, 81, (2022) 105332, ISSN 0887-2333, https://doi.org/10.1016/j.tiv.2022.105332. IF 3.18 (2020)

Ciffroy P, Mertens B, Van Hoeck E, Van Overmeire I, Johansson E, Alfonso B, Baderna D, Selvestrel G, Benfenati E

Modeling the migration of chemicals from food contact materials to food: The MERLIN-expo/VERMEER toolbox,

Food and Chemical Toxicology, 166 (2022) 113118, https://doi.org/10.1016/j.fct.2022.113118. IF 5.572 (2021)

Delre P, Lavado GJ, Lamanna G, Saviano M, Roncaglioni A, Benfenati E, Mangiatordi GF, Gadaleta D

Ligand-based prediction of hERG-mediated cardiotoxicity based on the integration of different machine learning techniques

Frontiers in Pharmacology, 13 (2022), DOI=10.3389/fphar.2022.951083 IF 5.988

Escher SE, Aguayo-Orozco A, Benfenati E, Bitsch A, Braunbeck T, Brotzmann K, Bois F, van der Burg B, Castel J, Exner T, Gadaleta D, Gardner I, Goldmann G, Hatley O, Golbamaki N, Graepel R, Jennings P, Limonciel A, Long A, Maclennan R, Mombelli E, Norinder U, Jain S, Santos Capinha L, Taboureau OT, Tolosa L, Vrijenhoek NG, van Vugt-Lussenburg BMA, Walker P, van de Water B, Wehr M, White A, Zdrazil B, Fisher C,

Integrate mechanistic evidence from new approach methodologies (NAMs) into a read-across assessment to characterise trends in shared mode of action,

Toxicology in Vitro, 79 (2022) 105269, ISSN 0887-2333, https://doi.org/10.1016/j.tiv.2021.105269. IF 3.18 (2020)

Gadaleta D, Spînu N, Roncaglioni A, Cronin M, Benfenati E.

Prediction of the Neurotoxic Potential of Chemicals Based on Modelling of Molecular Initiating Events Upstream of the Adverse Outcome Pathways of (Developmental) Neurotoxicity.

International journal of molecular sciences, 23(6), 2022) 3053. https://doi.org/10.3390/ijms23063053 IF 5.924 (2020)

Golbamaki A, Benfenati E

In silico methods for carcinogenicity assessment.

Methods in Molecular Biology 2425 (2022) 201-216. Benfenati E (Ed.). In silico Methods for Predicting Drug Toxicity. Second Edition. Springer, New York, USA

Khan K, Kumar V, Colombo E, Lombardo A, Benfenati E, Roy K.

Intelligent consensus predictions of bioconcentration factor of pharmaceuticals using 2D and fragment-based descriptors.

Environ Int. 2022 Dec;170:107625. doi: 10.1016/j.envint.2022.107625.

Lavado GJ, Baderna D, Carnesecchi E, Toropova AP, Toropov AA, Dorne JLCM, Benfenati E

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 IF 10.39 (2020)

Lombardo A, Manganaro A, Arning J, Benfenati E

Development of new QSAR models for water, sediment, and soil half-life,

Science of The Total Environment, Volume 838 (2022) 156004,ISSN 0048-9697, https://doi.org/10.1016/j.scitotenv.2022.156004

Luconi M, Sogorb MA, Markert UR, Benfenati E, May T, Wolbank S, Roncaglioni A, Schmidt A, Straccia M, Tait S. Human-Based New Approach Methodologies in Developmental Toxicity Testing: A Step Ahead from the State of the Art with a Feto–Placental Organ-on-Chip Platform.

International Journal of Environmental Research and Public Health. 2022; 19(23):15828. https://doi.org/10.3390/ijerph192315828

Manganelli S, Gamba A, Colombo E, Benfenati E

Using VEGAHUB within a weight-of -evidence strategy.

Methods in Molecular Biology 2425. (2022) 305-324. Benfenati E (Ed.). In silico Methods for Predicting Drug Toxicity. Second Edition. Springer, New York, USA

Marzo M, Roncaglioni R, Kulkarni S, Barton-Maclaren TS, Benfenati E

In silico model for developmental toxicity

Methods in Molecular Biology 2425. (2022) 139-162. Benfenati E (Ed.). In silico Methods for Predicting Drug Toxicity. Second Edition. Springer, New York, USA

Mombelli E, Raitano G, Benfenati E

In silico prediction of chemically induced mutagenicity: a weight of evidence approach integrating information from QSAR and read-across predictions.

Methods in Molecular Biology 2425 (2022) 149-184. Benfenati E (Ed.). In silico Methods for Predicting Drug Toxicity. Second Edition. Springer, New York, USA

Pizzo F, Benfenati E

In silico models for repeated-dose toxicity (RTD): prediction of the noobserved adverse effect level (NOAEL) and lowest observed adverse effect level (LOAEL).

Methods in Molecular Biology 2425. (2022) 163-176. Benfenati E (Ed.). In silico Methods for Predicting Drug Toxicity. Second Edition. Springer, New York, USA

Roncaglioni A, Lombardo A, Benfenati A

The VEGAHUB platform: the philisophy and the tools

ATLA, 50 (2022). https://doi.org/10.1177/02611929221090530. IF 2.438

Selvestrel G, Lavado GJ, Toropova AP, Toropov AA, Gadaleta D, Marzo M, Baderna D, Benfenati E.

Monte Carlo Models for Sub-Chronic Repeated-Dose Toxicity: Systemic and Organ-Specific Toxicity.

International Journal of Molecular Sciences, 23(2022) 6615. https://doi.org/10.3390/ijms23126615

Tetko IV, Klambauer G, Clevert D-A, Shah I, Benfenati E

Artificial Intelligence Meets Toxicology

Chemical Research in Toxicology 2022 35, 1289-1290. DOI: 10.1021/acs.chemrestox.2c00196

Toropov AA, Di Nicola MR, Toropova AP, Roncaglioni A, Carnesecchi E, Kramer NI, Williams AJ, Ortiz-Santaliestra ME, Benfenati E, Dorne JLCM,

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, ISSN 0048-9697, https://doi.org/10.1016/j.scitotenv.2022.154795. Ij 7.96 (2020)

Toropova AP, Toropov AA, Lombardo A, Lavado G, Benfenati E

Paradox of 'ideal correlations': improved model for air half-life of persistent organic pollutants

Environmental Technology, 43:16, (2022) 2510-2515, DOI: 10.1080/09593330.2021.1882588

Toropova AP, Toropov AA, Roncaglioni A, Benfenati E

The system of self-consistent models for vapour pressure

Chemical Physics Letters 790 (2022) 139354. https://doi.org/10.1016/j.cplett.2022.139354

Toropova AP, Toropov AA, Roncaglioni A, Benfenati E

Monte Carlo technique to study the adsorption affinity of azo dyes by applying new statistical criteria of the predictive potential, SAR and QSAR in Environmental Research, (2022) DOI: 10.1080/1062936X.2022.2104369

Toropova AP, Toropov AA, Viganò EL, Colombo E, Roncaglioni A, Benfenati E

Carcinogenicity prediction using the index of ideality of correlation

SAR and QSAR in Environmental Research, 33:6 (2022), 419-428, DOI: 10.1080/1062936X.2022.2076736

Viganò EL, Colombo E, Raitano G, Manganaro A, Sommovigo A, Dorne JLC, Benfenati E. Virtual Extensive Read-Across: A New Open-Access Software for Chemical Read-Across and Its Application to the Carcinogenicity Assessment of Botanicals. Molecules. 2022 Oct 5;27(19):6605. doi: 10.3390/molecules27196605.

Zare Jeddi M, Hopf NB, Louro H, Viegas S, Galea KS, Pasanen-Kase R, Santonen T, Mustieles V, Fernandez MF, Verhagen H, Bopp SK, Antignac JP, David A, Mol H, Barouki R, Audouze K, Duca R-C, Fantke P, Scheepers P, Ghosh M, Van Nieuwenhuyse A, Lobo Vicente J, Trier X, Rambaud L, Fillol C, Denys S, Conrad A, Kolossa-Gehring M, Paini A, Arnot J, Schulze F, Jones K, Sepai O, Ali I, Brennan L, Benfenati E, Cubadda F, Mantovani A, Bartonova A, Connolly A, Slobodnik J, Bruinen de Bruin Y, van Klaveren J, Palmen N, Dirven H, Husøy T, Thomsen C, Virgolino A, Röösli M, Gant T, von Goetz N, Bessems J

Developing human biomonitoring as a 21st century toolbox within the European exposure science strategy 2020–2030,

Environment International, 168 (2022) 107476, https://doi.org/10.1016/j.envint.2022.107476.

2021

Baderna D, Faoro R, Selvestrel G, Troise A, Luciani D, Andres S, Benfenati E

Defining the Human-Biota Thresholds of Toxicological Concern for Organic Chemicals in Freshwater: The Proposed Strategy of the LIFE VERMEER Project Using VEGA Tools

Molecules. 2021 Mar 30;26(7):1928. doi: 10.3390/molecules26071928. IF 4.148

Dorne JLCM, Richardson J, Livaniou A, Carnesecchi E, Ceriani L, Baldin R, Kovarich S, Pavan M, Saouter E, Biganzoli F, Pasinato L, Zare Jeddi M, Robinson TP, Kass GEN, Liem AKD, Toropov AA, Toropova AP, Yang C, Tarkhov A, Georgiadis N, Di Nicola MR, Mostrag A, Verhagen H, Roncaglioni A, Benfenati E, Bassan A,

EFSA's OpenFoodTox: An open source toxicological database on chemicals in food and feed and its future developments,

Environment International, 146, 2021, 106293, ISSN 0160-4120, https://doi.org/10.1016/j.envint.2020.106293. IF 9.621

EFSA Scientific Committee, More SJ, Bampidis V, Benford D, Hougaard Bennekou S, Bragard C, Halldorsson TI, Hernández-Jerez AF, Koutsoumanis K, Naegeli H, Schlatter JR, Silano V, Saxmose Nielsen S, Schrenk D, Turck D, Younes M, Benfenati E, Castle L, Cedergreen N, Hardy A, Laskowski R, Leblanc JC, Kortenkamp A, Ragas A, Posthuma L, Svendsen C, Solecki R, Testai E, Dujardin B, Kass GEN, Manini P, Zare Jeddi M, Dorne JLCM, Hogstrand C

Guidance on harmonised methodologies for human health, animal health and ecological risk assessment of combined exposure to multiple chemicals

EFSA Journal, 2021. https://doi.org/10.2903/j.efsa.2021.7033

Escher SE, Aguayo-Orozco A, Benfenati E, Bitsch A, Braunbeck T, Brotzmann K, Bois F, van der Burg B, Castel J, Exner T, Gadaleta D, Gardner I, Goldmann D, Hatley O, Golbamaki N, Graepel R, Jennings P, Limonciel A, Long A, Maclennan R, Mombelli E, Norinder U, Jain S, Santos Capinha L, Taboureau OT, Tolosa L, Vrijenhoek NG, van Vugt-Lussenburg BMA, Walker P, van de Water B, Wehr M, White A, Zdrazil B, Fisher C

Integrate mechanistic evidence from new approach methodologies (NAMs) into a read-across assessment to characterise trends in shared mode of action

Toxicology in Vitro, 79, 2022, 105269, ISSN 0887-2333, https://doi.org/10.1016/j.tiv.2021.105269. IF 3.18 (2020)

Gadaleta D, Benfenati E

A descriptor-based analysis to highlight the mechanistic rationale of mutagenicity

J Environ Sci Health C Toxicol Carcinog. (2021) May 6;1-24. doi: 10.1080/26896583.2021.1883964 IF 3.781

Gadaleta D, d'Alessandro L, Marzo M, Benfenati E, Roncaglioni A

Quantitative Structure-Activity Relationship Modeling Of The Amplex Ultrared (AUR) Assay To Predict Tyroperoxidase Inhibitory Activity

Frontiers in Pharmacology, section Predictive Toxicology. doi.org/10.3389/fphar.2021.713037. IF 5.81

Gadaleta D, Marzo M, Toropov A, Toropova A, Lavado G, Escher S, Dorne JL, 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://dx.doi.org/10.1021/acs.chemrestox.0c00176

IF 3.184

Kar S, Sanderson H, Roy K, Benfenati E, Leszczynski J

Green Chemistry in the Synthesis of Pharmaceuticals

Chem Rev, 2021. https://doi.org/10.1021/acs.chemrev.1c00631. IF 60.62

Lavado G J., Baderna D, Gadaleta D, Ultre M, Roy K, Benfenati E

Ecotoxicological QSAR modeling of the acute toxicity of organic compounds to the freshwater crustacean Thamnocephalus platyurus

Chemosphere 280 (2021) 130652, https://doi.org/10.1016/j.chemosphere.2021.130652. IF 7.086

Mansouri K, Karmaus AL, Fitzpatrick J, Patlewicz G, Pradeep P, Alberga D, Alepee N, Allen TEH, Allen D, Alves VM, Andrade CH, Auernhammer TR, Ballabio D, Bell S, Benfenati E, Bhattacharya S, Bastos JV, Boyd S, Brown JB, Capuzzi SJ, Chushak Y, Ciallella H, Clark AM, Consonni V, Daga PR, Ekins S, Farag S, Fedorov M, Fourches D, Gadaleta D, Gao F, Gearhart JM, Goh G, Goodman JM, Grisoni F, Grulke CM, Hartung T, Hirn M, Karpov P, Korotcov A, Lavado GJ, Lawless M, Li X, Luechtefeld T, Lunghini F, Mangiatordi GF, Marcou G, Marsh D, Martin T, Mauri A, Muratov EN, Myatt GJ, Nguyen D-T, Nicolotti O, Note R, Pande P, Parks AK, Peryea T, Polash AH, Rallo R, Roncaglioni A, Rowlands C, Ruiz P, Russo DP, Sayed A, Sayre R, Sheils T, Siegel C, Silva AC, Simeonov A, Sosnin S, Southall N, Strickland J, Tang Y, Teppen B, Tetko IV, Thomas D, Tkachenko V, Todeschini R, Toma C, Tripodi I, Trisciuzzi D, Tropsha A, Varnek A, Vukovic K, Wang Z, Wang L, Waters KM, Wedlake AJ, Wijeyesakere SJ, Wilson D, Xiao Z, Yang H, Zahoranszky-Kohalmi G, Zakharov AV, Zhang FF, Zhang Z, Zhao T, Zhu H, M. Zorn KM, Casey W, Kleinstreuer NC

CATMoS: Collaborative Acute Toxicity Modeling Suite

Environmental Health Perspectives 129 (2021) 047013. 9,031

Selvestrel G, Robino F, Baderna D, Manganelli S, Asturiol D, Manganaro A, Zanotti Russo M, Lavado G, Toma C, Roncaglioni A, Benfenati E.

SpheraCosmolife: a new tool for the risk assessment of cosmetic products

ALTEX - Alternatives to animal experimentation, 2021, 38(4), 565-579. doi: 10.14573/altex.2010221. IF 6.043 (2020)

Tan H, Chen Q, Hong H, Benfenati E, Gini GC, Zhang X, Yu H, Shi W

Structures of Endocrine-Disrupting Chemicals Correlate with the Activation of 12 Classic Nuclear Receptors

Environ. Sci. Technol. 2021, 55, 24, 16552–16562 doi.org/10.1021/acs.est.1c04997

Toma C, Cappelli CI, Manganaro A, Lombardo A, Arning J, Benfenati E.

New Models to Predict the Acute and Chronic Toxicities of Representative Species of the Main Trophic Levels of Aquatic Environments.

Molecules 2021, 26, 6983. https://doi.org/10.3390/molecules26226983. IF 4.411

Toma C, Manganaro A, Raitano G, Marzo M, Gadaleta D, Baderna D, Roncaglioni A, Kramer N, Benfenati E.

QSAR Models for Human Carcinogenicity: An Assessment Based on Oral and Inhalation Slope Factors.

Molecules 2021, 26, 127. https://doi.org/10.3390/molecules26010127. IF 4.411

Toropov AA, Toropova AP, Benfenati E

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

Toropov AA, Toropova AP, Marzo M, Carnesecchi, E, Selvestrel G, Benfenati E

Pesticides, cosmetics, drugs: identical and opposite influences of various molecular features as measures of endpoints similarity and dissimilarity.

Mol Divers 25, 1137–1144 (2021). https://doi.org/10.1007/s11030-020-10085-3

Toropov AA, Toropova AP, Roncaglioni A, Benfenati E,

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

Toropova AP, Toropov AA, Benfenati E
The self-organizing vector of atom-pairs proportions: use to develop models for melting points

Structural Chemistry, STUC-D-21-00146R2. IF 1.69

Toropova AP, Toropov AA, Lombardo A, Lavado G, Benfenati E

Paradox of 'ideal correlations': Improved model for air half-life of persistent organic pollutants.

Environmental Technology, 2021, https://doi.org/10.1080/09593330.2021.1882588

Toropova AP, Toropov AA, Lombardo A, Roncaglioni A, Lavado G, Benfenati E

The Monte Carlo method to build up models of the hydrolysis half-lives of organic compounds

SAR QSAR Environ Res. (2021) doi: 10.1080/1062936X.2021.1914156.

Toropova AP, Toropov AA, Roncaglioni A, Benfenati E

The index of ideality of correlation can improve the predictive potential of models of the antioxidant capacity of tripeptides from frog skin (Litoria rubella)

Computers in Biology and Medicine, 2021, 133, 104370

Vinken M, Benfenati E, Busquet E, Castell J, Clevert D-A, de Kok T, Dirven H, Fritsche E, Geris L. Gozalbes R, Hartung T, Jennen D, Jover R, Kandarova H, Kramer N, Krul C, Luechtefeld T, Masereeuw R, Roggen E, Schaller S, Vanhaecke T, Yang C, Piersma AH.

Safer chemicals using less animals: kick-off of the European ONTOX project.

Toxicology 458. 2021, 152846 (IF: 4.221).

Zare Jeddi M, Hopf NB, Viegas S, Bal Price A, Paini A, van Thriel C, Benfenati E, Ndaw S, Bessems J, Behnisch PA, Leng G, Duca R-C, Verhagen H, Cubadda F, Brennan L, Ali I, David A, Mustieles V, Fernandez MF, Louro H, Pasanen-Kase R.

Towards a systematic use of effect biomarkers in population and occupational biomonitoring,

Environment International, 146, 2021, 106257, ISSN 0160-4120, https://doi.org/10.1016/j.envint.2020.106257. IF 9.621

2020

Baderna D, Gadaleta D, Lostaglio E, Selvestrel G, Raitano G, Golbamaki A, Lombardo A, Benfenati E

New in silico models to predict in vitro micronucleus induction as marker of genotoxicity

Journal Hazardous Material, 2020, 385, 121638, https://doi.org/10.1016/j.jhazmat.2019.121638

IF: 9.038

Benfenati E, Carnesecchi E, Roncaglioni A, Baldin R, Ceriani L, Ciacci A, Kovarich S, Sartori L, Mostrag A, Magdziarz T, Yang C

Maintenance, update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0

EFSA Journal 2020; EN-1822: 1-36. https://doi.org/10.2903/sp.efsa.2020.EN-1822

Cappelli CI, Manganelli, Toma C, Emilio Benfenati E, Mombelli E

Prediction of the Partition Coefficient between Adipose Tissue and Blood for Environmental Chemicals: from Single

QSAR Models to an Integrated Approach

Mol. Inf. 2020, 39, 2000072, DOI: 10.1002/minf.202000072

Cappelli CI, Toropov AA, Toropova A, Benfenati E

Ecosystem ecology: Models for acute toxicity of pesticides towards Daphnia magna

Environemntal Toxicology and Pharmacology, 2020, 80, 103459. https://doi.org/10.1016/j.etap.2020.103459

IF 3.292

Carnesecchi E, Raitano G, Gamba A, Benfenati E, Roncaglioni A

Evaluation of non-commercial models for genotoxicity and carcinogenicity in the assessment of EFSA's databases

SAR and QSAR in Environmental Research, 2020, 31, 33-48. doi: 10.1080/1062936X.2019.1690045.

IF 2.053

Carnesecchi E, Toma C, Roncaglioni A, Kramer N, Benfenati E, Dorne JLCM

Integrating QSAR models predicting acute contact toxicity and mode of action profiling in honey bees (A. mellifera): Data curation using open source databases, performance testing and validation

Science of The Total Environment, Volume 735, 15 September 2020, 139243.
https://doi.org/10.1016/j.scitotenv.2020.139243

IF 6.511

Carnesecchi E, Toropov AA, Toropova AP, Kramer N, Svendsen C, Dorne JL, Benfenati E

Predicting acute contact toxicity of organic binary mixtures in honey bees (A. mellifera) through innovative QSAR models
Science of the Total Environment, 2020, 704, 135302, https://doi.org/10.1016/j.scitotenv.2019.135302

IF 6.511

Chayawan, Cosimo Toma, Emilio Benfenati, Ana Yisel Caballero Alfonso

Towards an understanding of the mode of action of human aromatase activity for azoles through quantum-chemical descriptors-based regression and SAR modelling analysis

Molecules, (2020), *25*(3), 739; https://doi.org/10.3390/molecules25030739

IF 3.267

EFSA Panel on Food Contact Materials, Enzymes and Processing Aids (CEP), Silano V, Barat Baviera JM, Bolognesi C, Chesson A, Cocconcelli PS, Crebelli R, Gott DM, Grob K, Lambré C, Lampi E, Mengelers M, Mortensen A, Steffensen I-L, Tlustos C, Van Loveren H, Vernis L, Zorn H, Benfenati E, Castle L, Di Consiglio E, Franz F, Hellwig N, Milana MR, Pfaff K, Civitella C, Lioupis A, Pizzo F, Rivière G

Review and priority setting for substances that are listed without a specific migration limit in Table 1 of Annex 1 of Regulation 10/2011 on plastic materials and articles intended to come into contact with food

EFSA Journal 2020, 18, e06124. https://doi.org/10.2903/j.efsa.2020.6124

Gadaleta D, Golbamaki Bakhtyari A, Lavado GJ, Roncaglioni A, Benfenati E.

Automated integration of structural, biological and metabolic similarities to improve read-across

ALTEX - Alternatives to animal experimentation, 2020, 37(3), 469-481. doi: 10.14573/altex.2002281.

IF 5.787

Ghosh S, Ojha PK, Carnesecchi E, Lombardo A, Roy K, Benfenati E

Exploring QSAR modeling of toxicity of chemicals on earthworm

Ecotoxicology and Environmental Safety, 2020, 190, 110067, https://doi.org/10.1016/j.ecoenv.2019.110067

IF 4.782

Kar S, Sanderson H, Roy K, Benfenati E, Leszczynski J

Ecotoxicological assessment of pharmaceuticals and personal care products using predictive toxicology approaches

Green Chemistry, 2020, 22, 1458 – 1516 DOI: 10.1039/C9GC03265G

IF 9.405

Khan PM, Baderna D, Lombardo A, Roy K, Benfenati E

Chemometric modeling to predict air half-life of persistent organic pollutants (POPs)

Journal of Hazardous Materials, 2020, 382, 121035. https://doi.org/10.1016/j.jhazmat.2019.121035

IF: 9.038

Lavado GJ, Baderna D, Gadaleta D, Ultre M, Roy K, Benfenati E

Ecotoxicological QSAR modeling of the acute toxicity of organic compounds to the freshwater crustacean Thamnocephalus platyurus

Chemosphere 280 (2021) 130652

Lavado G, Toropova AP, Toropov AA, Golbamaki A, Toma C, Gadaleta D, Benfenati E, Marzo M

Zebrafish AC50 Modelling: (Q)SAR models to predict developmental toxicity in zebrafish embryo

Ecotoxicology and Environmental Safety, 2020, 110936. doi.org/10.1016/j.ecoenv.2020.110936

IF 4.872

Manganelli S, Schilter B, Scholz G, Benfenati E, Lo Piparo E

Value and limitation of structure-based profilers to characterize developmental and reproductive toxicity potential.

Arch Toxicol, 2020, 94, 939–954. https://doi.org/10.1007/s00204-020-02671-z

IF 5.059

Mansouri K, Kleinstreuer N, Abdelaziz A M., Alberga D, Alves V M., Andersson P L., Andrade C H., Bai F, Balabin I, Ballabio D, Bay Benfenati E, Bhhatarai B, Boyer S, Chen J, Consonni V, Farag S, Fourches D, García-Sosa A T., Gramatica P, Grisoni F, Grulke C M., Hong H, Horvath D, Hu X, Huang R, Jeliazkova N, Li J, Li X, Liu H, Manganelli S, Mangiatordi G, Maran U, Marcou G, Martin T, Muratov E, Nguyen D-T, Nicolotti O, Nikolov G. N, Norinder U, Papa E, Petitjean M, Piir G, Poroikov V, Qiao X, Richard A M., Roncaglioni A, Ruiz P, Rupakheti C, Sakkiah S, Sangion A, Schramm K-W, Selvaraj C, Shah I, Sild S, Sun L, Taboureau O, Tang Yun, Tetko Igor, Todeschini Roberto, Tong Weida, Trisciuzzi Daniela, Tropsha Alexander, VanDenDriessche George, Varnek A, Wang Z, Wedebye E, Williams A J., Xie H, Zakharov A, Zheng Z, Judson R S.

CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity

Environ Health Perspectives, 2020, 128, 027002, https://doi.org/10.1289/EHP5580

IF 8.382

Marzo M, Lavado GJ, Como F, Toropov AA, Toropova AP, Baderna D, Cappelli C, Lombardo A, Toma C,

Blázquez Sánchez M, Benfenati E

QSAR models for Biocides. The example of the prediction of Daphnia magna acute toxicity

SAR and QSAR Environ Research, 2020, 31, 227-243, https://doi.org/10.1080/1062936X.2019.1709221

IF 2.053

Mora Lagares L, Minovski , N, Caballero Alfonso AY , Benfenati E, Wellens S, Culot M, Fabien Gosselet F, Novič M

Homology Modelling of the Human P-glycoprotein (ABCB1) and Insights into Ligand Binding Through Molecular Docking Studies

Int J Mol Sci, 2020, 21(11):4058. doi: 10.3390/ijms21114058.

IF 4.556

Rogiers V, Benfenati E, Bernauer U, Bodin L, Carmichael P, Chaudhry Q, Coenraads PJ, Cronin MTD, Dent M, Dusinska M, Ellison C, Ezendam J, Gaffet E, Galli CL, Goebel C, Granum B, Hollnagel HM, Kern PS, Kosemund-Meynen K, Ouédraogo G, Panteri E, Rousselle C, Stepnik M, Vanhaecke T, von Goetz N, Worth A

The way forward for assessing the human health safety of cosmetics in the EU workshop proceed

Toxicology, 2020, 436, 152421, https://doi.org/10.1016/j.tox.2020.152421

IF 4.099

Rovida C, Barton-Maclaren T, Benfenati E, Caloni F, Chandrasekera C, Chesne C, Cronin MTD, De Knech Jt, Dietrich DR, Escher SE, Fitzpatrick S, Flannery B, Herzler M, Hougaard Bennekou S, Hubesch B, Kamp H, Kass G, Kisitu J, Kleinstreuer N, Kovarich S, Leist M, Maertens A, Nugent K, Pallocca G, Pastor M, Patlewicz G, Pavan M, Richarz A, Smirnova L, Schwarz M, Yamada T, Hartung T

t4 workshop report. Internationalisation of read-across as a validated new approach method (NAM) for regulatory toxicology

ALTEX, 2020 **DOI** https://doi.org/10.14573/altex.1912181

IF 5.787

Roy J, Ojha PK, Carnesecchi E, Lombardo A, Roy K, Benfenati E

First report on a classification-based QSAR model for chemical toxicity to earthworm

Journal of Hazardous Materials, 2020, 386: 121660, https://doi.org/10.1016/j.jhazmat.2019.121660

IF 9.038

Sauer UG, Barter RA, Becker RA, Benfenati E, Berggren E, Hubesch B, Hollnagel HM, Inawaka K, Keene AM, Mayer P, Plotzkel K, Skoglund R, Albert O

21st Century Approaches for Evaluating Exposures, Biological Activity, and Risks of Complex Substances: Workshop highlights

Regulatory Toxicology and Pharmacology, 2020, 111, 104583. https://doi.org/10.1016/j.yrtph.2020.104583

IF 2.652

Silano V, Barat Baviera JM, Bolognesi C, Chesson A, Cocconcelli PS, Crebelli R, Gott DM, Grob K, Lambr_e C, Lampi E, Mengelers M, Mortensen A, Steffensen I-L, Tlustos C, Van Loveren H, Vernis L, Zorn H, Benfenati E, Castle L, Di Consiglio E, Franz R, Hellwig N, Milana MR, Pfaff K, Civitella C, Lioupis A, Pizzo F and Rivière G, 2020. Scientific Opinion on the review and priority setting for substances that are listed without a specific migration limit in Table 1 of Annex 1 of Regulation 10/2011 on plastic materials and articles intended to come into contact with food. EFSA Journal 2020;18(6):6124, 104 pp. https://doi.org/10.2903/j.efsa.2020.6124

Tan H, Wang X, Hong H, Benfenati E, Giesy J P, Gini G, Kusko R , Zhang X, Yu H, Shi W

Structures of endocrine-disrupting chemicals determine binding to and activation of the estrogen receptor α and androgen receptor

Environ Sci Technol 2020 ; 54 : 11424-11433

IF: 7.864

Toropov AA, Toropova AP, Benfenati E

QSAR model for pesticides toxicity to Rainbow Trout based on “ideal correlations”.

Aquatic Toxicology, 227, 2020, 105589. https://doi.org/10.1016/j.aquatox.2020.105589

IF 4.344

Toropov AA, Toropova AP, Benfenati E

"Ideal correlations" for the predictive toxicity to Tetrahymena pyriformis.

Toxicology Mechanisms and Methods, 30(8), 2020, 605-610.

Toropov AA, Toropova AP, Carnesecchi E, Benfenati E, Dorne JL

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 https://doi.org/10.1007/s11224-020-01525-9

IF 2.081

Toropov AA, Toropova AP, Marzo M, Benfenati E

Use of the Index of Ideality of Correlation to improve aquatic solubility model

Journal of Molecular Graphics and Modelling, 2020, 96, 107525.
https://doi.org/10.1016/j.jmgm.2019.107525

IF 2.079

Toropov AA, Toropova AP, Selvestrel G, Baderna D, Benfenati E

Prediction of No Observed Adverse Effect Concentration for Inhalation toxicity: Monte Carlo approach.

SAR and QSAR in Environmental Research, 31(12), 2020, 1-12.

Toropova AP, Toropov AA, Benfenati E

QSAR-models, validation, and IIC-paradox for drug toxicity

International Journal of Quantitative Structure-Property Relationships, 2020, 5, 22-43. DOI: 10.4018/IJQSPR.2020010102

Toropova AP, Toropov AA, Carnesecchi E, Benfenati E, Dorne JL

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. https://doi.org/10.1007/s11356-020-07820-6

IF 3.056

Toropova AP, Toropov AA, Carnesecchi E, Benfenati E, Dorne JL

The index of ideality of correlation: models for flammability of binary liquid mixtures.

Chemical Papers, 2020, 74(2): 601-609. https://doi.org/10.1007/s11696-019-00903-w

IF 1.68

Van Bossuyt M, Raitano G, Honma M, Van Hoeck E, Vanhaecke T, Rogiers V, Mertens B, Benfenati E

New QSAR models to predict chromosome damaging potential based on the in vivo micronucleus test

Toxicology Letters, 2020, 329:80-84, DOI: 10.1016/j.toxlet.2020.04.016

IF 3.569

Volta A, Sforzini S, Camurati C, Teoldi F, Maiorana S, Croce A, Benfenati E, Perricone G, Lodi M, Viarengo A

Ecotoxicological effects of atmospheric particulate produced by braking systems on aquatic and edaphic organisms

Environment International, 2020, 137, 105564. https://doi.org/10.1016/j.envint.2020.105564

IF 7.577

2019

Baderna D, Caloni F, Benfenati E

Investigating landfill leachate toxicity in vitro: A review of cell models and endpoints.

Environ Int. 2019 Jan;122:21-30. doi: 10.1016/j.envint.2018.11.024.

IF: 7.577

Benfenati E, Chaudhry Q, Gini G, Dorne JL

Integrating in silico models and read-across methods for predicting toxicity of chemicals: A step-wise strategy

Environment International 2019; 131, 105060, doi: 10.1016/j.envint.2019.105060

IF: 7.577

Blázquez M, Andreu-Sánchez O, Ranero I, Fernández-Cruz ML, Benfenati E

Comparing in vivo data and in silico predictions for acute effects assessment of biocidal active substances and metabolites for aquatic organisms,

Ecotoxicology and Environmental Safety, 205, 2020, 111291, ISSN 0147-6513, https://doi.org/10.1016/j.ecoenv.2020.111291.

Blazquez M, Fernandez-Cruz M L, Gajewicz A, Puzyn T, Benfenati E

On the uses of predictive toxicology to approve the use of engineered nanomaterials as biocidal active substances under the Biocidal Products Regulation

IOP Conference Series: Materials Science and Engineering 2019; 499: 012007

Caballero-Alfonso AY, Cruz-Monteagudo M, Tejera E, Benfenati E, Borges F, Cordeiro MNDS, Armijos-Jaramillo V, Perez-Castillo Y.

Ensemble-Based Modeling of Chemical Compounds with Antimalarial Activity.

Curr Top Med Chem. 2019;19:957-969. doi: 10.2174/1568026619666190510100313.

IF: 3.218

Carnesecchi E, Svendsen C, Lasagni S, Grech A, Quignot N, Amzal B, Toma C, Tosi S, Rortais A, Cortinas-Abrahantes J, Capri E, Kramer N, Benfenati E, Spurgeon D, Guillot G, Dorne JLCM

Investigating combined toxicity of binary mixtures in bees: Meta-analysis of laboratory tests, modelling, mechanistic basis and implications for risk assessment

Environment International, 2019, 133, 105256, https://doi.org/10.1016/j.envint.2019.105256

IF: 7.577

Gadaleta D, Vuković K, Toma C, Lavado G, Karmaus AL, Mansouri K, Kleinstreuer NC, Benfenati E, Roncaglioni A

SAR and QSAR modeling of a large collection of LD50 rat acute oral toxicity data

J Cheminform (2019) 11:58 https://doi.org/10.1186/s13321-019-0383-2

IF: 5.318

Gini G, Ferrari T, Lombardo A, Cassano A, Benfenati E

A New QSAR Model for Acute Fish Toxicity based on Mined Structural Alerts

Journal of Toxicology and Risk Assessment, 5: 016 (2019) DOI: 10.23937/2572-4061.1510016

Gini G, Zanoli F, Gamba A, Raitano G, Benfenati E

Could deep learning in neural networks improve the QSAR models?

SAR and QSAR in Environmental Research, 2019, Vol 30, Pages 617-642 DOI: 10.1080/1062936x.2019.1650827

IF: 2.053

Honma M, Kitazawa A, Cayley A, Williams R, Barber, Hanser, Saiakhov R, Chakravarti S, Myatt G J, Cross K P, Benfenati E, Raitano G, Mekenyan O, Petkov P, Bossa C, Benigni R, Battistelli C L, Giuliani A, Tcheremenskaia O, DeMeo C, Norinder U, Koga H, Jose C, Jelazkova N, Kochev N, Paskaleva V, Yang C, Daga P R, Clark R D, Rathman J

Improvement of quantitative structure-activity relationship (QSAR) tools for predicting Ames mutagenicity: outcomes of the Ames/QSAR International Challenge Project

Mutagenesis 2019,34:3-16. doi: 10.1093/mutage/gey031

IF: 3.379

Khan K, Baderna D, Cappelli C, Toma C, Lombardo A, Roy K, Benfenati E

Ecotoxicological QSAR modeling of organic compounds against fish: Application of fragment based descriptors in feature analysis

Aquatic Toxicology, 2019 212, 162-174, https://doi.org/10.1016/j.aquatox.2019.05.011

IF: 4.344

Khan K, Benfenati E, Roy K

Consensus QSAR modeling of toxicity of pharmaceuticals to different aquatic organisms: Ranking and prioritization of the DrugBank database compounds

Ecotoxicology and Environmental Safety 168 (2019) 287–297

IF: 4.872

Khan K, Khan PM, Lavado G, Valsecchi C, Pasqualini J, Baderna D, Marzo M, Lombardo A, Roy K, Benfenati E

QSAR modeling of Daphnia magna and fish toxicities of biocides using 2D descriptors

Chemosphere, 2019, 229, 8-17, https://doi.org/10.1016/j.chemosphere.2019.04.204

IF: 5.778

Khan K, Roy K, Benfenati E

Ecotoxicological QSAR modeling of endocrine disruptor chemicals

J Hazard Mater 2019; 369 : 707-718 DOI:10.1016/j.jhazmat.2019.02.019

IF: 9.038

Khan PM, Roy K, Benfenati E

Chemometric modeling of Daphnia magna toxicity of agrochemicals

Chemosphere 2019, 224, 470-479, https://doi.org/10.1016/j.chemosphere.2019.02.147

Maiorana S, Teoldi F, Silvani S, Mancini A, Sanguineti A, Mariani F, Cella C, Lopez A, Potenza M A C, Lodi M, Dupin D, Sanvito T, Bonfanti A, Benfenati E, Baderna D

Phytotoxicity of wear debris from traditional and innovative brake pads

Environ Int 2019 ; 123 : 156-163 https://doi.org/10.1016/j.envint.2018.11.057

IF: 7.577

Manganelli S, Roncaglioni A, Mansouri K, Judson R S, Benfenati E, Manganaro A, Ruiz P

Development, validation and integration of in silico models to identify androgen active chemicals

Chemosphere 2019; 220 : 204-215 doi: 10.1016/j.chemosphere.2018.12.131

IF: 5.778

Marzo M, Leone C, Toma C, Roncaglioni A, Gianazzi S, Knauf R, Benfenati E

Impact of REACH legislation on the production and importation of CMR (carcinogen, mutagen and reproductive) and explosive chemicals in Italy from 2011 to 2015

Regul Toxicol Pharmacol 2019; 101 : 166-171 doi: 10.1016/j.yrtph.2018.11.013

IF: 2.652

More SJ, Hardy A, Bampidis V, Benford D, Hougaard Benneku S, Bragard C, J. Boesten J, T. I. Halldorsson TI, A. F. Hernadez-Jerez AF , M. J. Jeger MJ, H. K. Knutsen HK, K. P. Koutsoumanis KP, H. Naegeli H , H. Noteborn H , C. Ockleford C, A. Ricci A, G. Rychen G, J R Schlatter JR, V. Silano V, S S Nielsen SS, D. Schrenk D, Solecki R, Turck D, Younes M, Benfenati E, Castle L, Cedergreen N, Svendsen C, Testai E, Dujardin B, Kass GEN, Manini P, Jeddi MZ, Dorne JLCM, Hogstrand C.

Guidance on harmonized methodologies for human health, animal health and ecological risk assessment of contributed exposure to multiple chemicals.

EFSA Journal 2019, 17, 5634. Doi: 10.2903/J.efsa.2019.5634

Raitano G, Roncaglioni A, Manganaro A, Honma M, Sousselier L, Do Q-T, Paya E, Benfenati E

Integrating in silico models for the prediction of mutagenicity (Ames test) of botanical ingredients of cosmetics.

Computational Toxicology, DOI: 10.1016/j.comtox.2019.100108

Toma C, Gadaleta D, Roncaglioni A, Toropov A A, Toropova A P, Marzo M, Benfenati E

QSAR development for plasma protein binding: Influence of the ionization state

Pharm Res 2019; 36: 28

IF: 3.242

Toropov A A, Toropova A P, Benfenati E

The Index of Ideality of Correlation: QSAR model of acute toxicity for zebrafish (Danio rerio) embryo

Int J Environ Res 2019; 13: 387-394

IF: 2.007

Toropov AA, Toropova AP, Raitano G, Benfenati E

CORAL: building up QSAR models for the chromosome aberration test.

Saudi Journal of Biological Sciences, 2019: 26: 1101-1106. https://doi.org/10.1016/j.sjbs.2018.05.013

IF: 2.802

Toropov AA, Toropova AP, Selvestrel G, Benfenati E

Idealization of correlations between optimal simplified molecular input-line entry system-based descriptors and skin sensitization

SAR and QSAR in Environmental Research, 2019, 30, 447-455, https://doi.org/10.1080/1062936X.2019.1615547

IF: 2.053

Toropova A P, Toropov A A, Benfenati E

Semi-correlations as a tool to build up categorical (active/inactive) model of GABAA receptor modulator activity

Struct Chem 2019; 30: 853-861

IF: 2.081

Toropova AP, Toropov AA, Benfenati E

QSPR as a random event: solubility of fullerenes C[60] and C[70],

Fullerenes, Nanotubes and Carbon Nanostructures 2019 27, 816-821, https://doi.org/10.1080/1536383X.2019.1649659

IF: 1.648

Toropova A P, Toropov A A, Benfenati E, Leszczynska D, Leszczynksy J

Virtual screening of anti-cancer compounds: Application of Monte Carlo technique

Anticancer Agents Med Chem 2019; 19: 148-153

IF: 2.049

Vian M, Raitano G, Roncaglioni A, Benfenati E

In silico model for mutagenicity (Ames test), taking into account metabolism

Mutagenesis 2019; 34 : 41-48 doi: 10.1093/mutage/gey045.

IF: 3.379

Vukovic K, Gadaleta D, Benfenati E

Methodology of aiQSAR: a group-specific approach to QSAR modelling

J Cheminform 2019, 11:27, https://doi.org/10.1186/s13321-019-0350-y

IF: 5.318

2018

Benfenati E, Golbamaki Bakhtyari A, Raitano G, Roncaglioni A, Manganelli S, Lemke F, Norinder U, Lo Piparo E, Honma M, Manganaro A, Gini G

A large comparison of integrated SAR/QSAR models of the Ames test for mutagenicity

SAR QSAR Environ Res 2018 ; 29 : 591-611 . doi: 10.1080/1062936X.2018.1497702

Ferrari F, Lombardo A., Benfenati E.

QSARpy: A new flexible algorithm to generate QSAR models based on dissimilarities. The log Kow case study.

Science of the Total Environment. 2018; 637-638 : 1158-1165 doi: 10.1016/j.scitotenv.2018.05.072.

Gadaleta D, Lombardo A, Toma C, Benfenati E

A new semi-automated workflow for chemical data retrieval and quality checking for modeling applications

J Cheminform 2018 ; 10 : 60 https://doi.org/10.1186/s13321-018-0315-

Gadaleta D, Manganelli S, Roncaglioni A, Toma C, Benfenati E, Mombelli E

QSAR modeling of toxcast assays relevant to the molecular initiating events of AOPs leading to hepatic steatosis

J Chem Inf Model 2018 ; 58 : 1501-1517 doi: 10.1021/acs.jcim.8b00297.

Golbamaki Bakhtyari A, Golbamaki Bakhtyari N, Sizochenko N, Rasulev B, Leszczynksy J, Benfenati E

Genotoxicity induced by metal oxide nanoparticles: a weight of evidence study and effect of particle surface and electronic properties

Nanotoxicology 2018 ; 12 : 1113-1129 doi: 10.1080/17435390.2018.1478999

Lombardo A, Raitano G, Gadaleta D, Benfenati E

Criteria and application on the use of nontesting methods within a weight of evidence strategy

Methods Mol Biol 2018 ; 1800 : 199-218 doi: 10.1007/978-1-4939-7899-1_9.

Manganelli S, Schilter B, Benfenati E, Manganaro A, Lo Piparo E

Integrated strategy for mutagenicity prediction applied to food contact chemicals

ALTEX 2018 ; 35 : 169-178 doi: 10.14573/altex.1707171.

Marzo M, Benfenati E

Classification of a Naïve Bayesian fingerprint model to predict reproductive toxicity

SAR QSAR Environ Res 2018 ; 29 : 631-645 https://doi.org/10.1080/1062936X.2018.1499125

Puzyn T, Jeliazkova N, Sarimveis H, Marchese Robinson R, Lobaskin V, Rallo R, Richarz A, Gajewicz A, Papadopulos M, Hastings J, Cronin M T D, Benfenati E, Fernandez A

Perspectives from the NanoSafety Modelling Cluster on the validation criteria for (Q)SAR models used in nanotechnology

Food Chem Toxicol 2018 ; 112 : 478-494. doi: 10.1016/j.fct.2017.09.037.

Raitano G, Goi D, Pieri V, Passoni A, Mattiussi M, Lutman A, Romeo I, Manganaro A, Marzo M, Porta N, Baderna D, Colombo A, Aneggi E, Natolino F, Lodi M, Bagnati R, Benfenati E

(Eco)toxicological maps: A new risk assessment method integrating traditional and in silico tools and its application in the Ledra River (Italy)

Environ Int 2018 ; 119 : 275-286 doi: 10.1016/j.envint.2018.06.035.

Toropova A P, Toropov A A, Benfenati E, Castiglioni S, Bagnati R, Passoni A, Zuccato E, Fanelli R

Quasi-SMILES as a tool to predict removal rates of pharmaceuticals and dyes in sewage

Process Saf Environ Prot 2018 ; 118 : 227-233 https://doi.org/10.1016/j.psep.2018.07.003

Toropov AA, Toropova AP, Roncaglioni A, Benfenati E

Prediction of Biochemical Endpoints by the CORAL Software: Prejudices, Paradoxes, and Results.

Methods in Molecular Biology, vol. 1800, Ch 27, Orazio Nicolotti (ed.), Computational Toxicology: Methods and Protocols, https://doi.org/10.1007/978-1-4939-7899-1_27, © Springer Science+Business Media, LLC, part of Springer Nature 2018.

Toropov AA, Toropova AP, Benfenati E, Diomede L, Salmona M

Use of Quasi-SMILES to model biological activity of "micelle-polymer" samples.

Struct Chem 2018 ; 29 : 1213-1223, DOI: 10.1007/s11224-018-1115-3

Toropova AP, Toropov AA, Benfenati E, Leszczynska D, Leszczynski J

Prediction of antimicrobial activity of large pool of peptides using quasi-SMILES.

Biosystems 2018 ; 169-170 : 5-12 doi: 10.1016/j.biosystems.2018.05.003.

Toropova AP, Toropov AA, Marzo M, Escher SE, Dorne JL, Georgiadis N, Benfenati E.

The application of new HARD-descriptor available from the CORAL software to building up NOAEL models.

Food and Chemical Toxicology, 112 (2018) 544-550. doi: 10.1016/j.fct.2017.03.060.

Toropov AA, Toropova AP, Benfenati E, Dorne JL

SAR for gastro-intestinal absorption and blood-brain barrier permeation of pesticides.

Chemico-Biological Interactions, 2018; 290 : 1-5. DOI: 10.1016/j.cbi.2018.04.030

Toropov AA, Toropova A P, Benfenati E, Salmona M

Mutagenicity, anticancer activity and blood brain barrier: similarity and dissimilarity of molecular alerts

Toxicol Mech Methods 2018 ; 28:5, 321-327. doi: 10.1080/15376516.2017.1422579.

Toropov A A, Toropova A P, Roncaglioni A, Benfenati E

Prediction of biochemical endpoints by the CORAL software: prejudices, paradoxes, and results

Methods Mol Biol 2018 ; 1800 : 573-583 doi: 10.1007/978-1-4939-7899-1_27.

Van Bossuyt M, Van Hoeck E, Raitano G, Vanhaecke T, Benfenati E, Mertens B, Rogiers V

Performance of in silico models for mutagenicity prediction of food contact materials

Toxicol Sci 2018 ; 163 : 632-638 doi: 10.1093/toxsci/kfy057.

2017

Toropov AA, Toropova AP, Cappellini L, Benfenati E, Davoli E

QSPR analysis of threshold of odor for the large number of heterogenic chemicals.

Molecular Diversity, Accepted: November 19, 2017. https://doi.org/10.1007/s11030-017-9800-5

Como F, Carnesecchi E, Volani S, Dorne J L, Richardson J C, Bassan A, Pavan M, Benfenati E

Predicting acute contact toxicity of pesticides in honeybees (Apis mellifera) through a k-nearest neighbor model

Chemosphere 2017; 166 : 438-444

Croce R, Cinà F, Lombardo A, Crispeyn G, Cappelli CI, Vian M, Maiorana S, Benfenati E, Baderna D.

Aquatic toxicity of several textile dye formulations: Acute and chronic assays with Daphnia magna and Raphidocelis subcapitata.

Ecotoxicol Environ Saf. 2017 Oct;144:79-87. doi: 10.1016/j.ecoenv.2017.05.046. Epub 2017 Jun 8.

Floris M, Raitano G, Medda, Benfenati E

Fragment Prioritization on a Large Mutagenicity Dataset

Molecular Informatics, 2017; 36: 1600133 ; DOI: 10.1002/minf.201600133

Gadaleta D, Porta N, Vrontaki E, Manganelli S, Manganaro A, Sello G, Honma M, Benfenati E.

Integrating computational methods to predict mutagenicity of aromatic azo compounds.

J Environ Sci Health C Environ Carcinog Ecotoxicol Rev. 2017 Oct 2;35(4):239-257. doi: 10.1080/10590501.2017.1391521. Epub 2017 Nov 27.

Golbamaki A, Franchi AM, Manganelli S, Manganaro A, Gini G, Benfenati E

ToxDelta: A New Program to Assess How Dissimilarity Affects the Effect of Chemical Substances

Drug Des, 2017, 6, 1000153. DOI: 10.4172/2169-0138.1000153

Hardy A, Benford D, Halldorsson T, Jeger MJ, Knutsen HK, More S, Naegeli H, Noteborn H, Ockleford C, Ricci A, Rychen G, Schlatter JR, Silano V, Solecki R, Turck D, Benfenati E, Chaudhry QM, Craig P, Frampton G, Greiner M, Hart A, Hogstrand C, Lambre C, Luttik R, Makowski D, Siani A, Wahlstroem H, Aguilera J, Dorne J-L, Dumon AFt, Hempen M, Valtena Martınez S, Martino l, Smeraldi C, Terron A, Georgiadis N, Younes M.

Guidance on the use of the weight of evidence approach in scientific assessments

EFSA Journal 2017; 15, 4971. doi: 10.2903/j.efsa.2017.4971

Hoang T, Castorina R, Gaspar F, Maddalena R, Jenkins P L, Zhang Q, McKone T E, Benfenati E, Shi A Y, Bradman A

VOC exposures in California early childhood education environments

Indoor Air 2017; 27: 609-621.

Manganelli S, Benfenati E.

Nano-QSAR Model for Predicting Cell Viability of Human Embryonic Kidney Cells.

Methods Mol Biol. 2017; 27:609-621. doi: 10.1007/978-1-4939-6960-9_22.

Negri E, Metruccio F, Guercio V, Tosti L, Benfenati E, Bonzi R, La Vecchia C, Moretto A

Exposure to PFOA and PFOS and fetal growth: A critical merging of toxicological and epidemiological data

Critical Reviews In Toxicology, 2017; 47(6):482-508. doi: 10.1080/10408444.2016.1271972

Raitano G, Benfenati E, Ananiadou S, Fu X, Do QT, Rat4P, Sousselier L

Role of in silico tools and text mining in the safety assessment of selected plant coumarins

Toxicology Letters 280S (2017) S92–S106

Richarz AN, Avramopoulos A, Benfenati E, Gajewicz A, Golbamaki Bakhtyari N, Leonis G, Marchese Robinson RL, Papadopoulos MG, Cronin MT, Puzyn T.

Compilation of Data and Modelling of Nanoparticle Interactions and Toxicity in the NanoPUZZLES Project.

Adv Exp Med Biol. 2017;947:303-324. doi: 10.1007/978-3-319-47754-1_10.

Teoldi F, Lodi M, Benfenati E, Colombo A, Baderna D

Air quality in the Olona Valley and in vitro human health effects

Sci Total Environ 2017 ; 579 : 1929-1939

Toropov AA, Toropova AP, Cappellini L, Benfenati E, Davoli E.

QSPR analysis of threshold of odor for the large number of heterogenic chemicals.

Mol Divers. 2017 Dec 5. doi: 10.1007/s11030-017-9800-5. [Epub ahead of print]

Toropov AA, Toropova AP, Marzo M, Dorne JK, Georgiadis G, Benfenati E

QSAR models for predicting acute toxicity of pesticides in rainbow trout using the CORAL software and EFSA's OpenFoodTox database

Environ. Pharmacol. Toxicol. 2017 ; 53: 158-163.

Van Bossuyt M, Van Hoeck E, Raitano G, Manganelli S, Braeken E, Ates G, Vanhaecke T, Van Miert S, Benfenati E , Mertens B, Rogiers V

(Q)SAR tools for priority setting: A case study with printed paper and board food contact material substances

Food and Chemical Toxicology, 2017. 102, 109-119.

2016

Ates G, Raitano G, Heymans A, Van Bossuyt M, Vanparys P, Mertens B, Chesne C, Roncaglioni A, Milushev D, Benfenati E, Rogiers V, Doktorova TY

In silico tools and transcriptomics analyses in the mutagenicity assessment of cosmetic ingredients: a proof-of-principle on how to add weight to the evidence

Mutagenesis, 2016, 31, 453-461. doi:10.1093/mutage/gew008

Benfenati E, Belli M, Borges T, Casimiro E, Cester J, Fernandez A, Gini G, Honma M, Kinzl M, Knauf R, Manganaro A, Mombelli E, Petoumenou MI, Paparella M, Paris P, Raitano G.

Results of a round-robin exercise on read-across

SAR and QSAR in Environmental Research, 2016, 27, 371-384

Benfenati E, Berggren E, Fritsche E, Hartung T, Slikker Jr W, Spielmann H, Testai E, Tice RR, Tiramani M, Villenave R

Novel chemical hazard characterisation approaches

EFSA Journal. Version of Record online: 30 JUN 2016 | DOI: 10.2903/j.efsa.2016.s0506

Gadaleta D, Manganelli S, Manganaro A, Porta N, Benfenati E

A knowledge-based expert rule system for predicting mutagenicity (Ames test) of aromatic amines and azo compounds

Toxicology 2016; 370: 20-30 IF 3.582

Golbamaki A, Benfenati E

In silico model for carcinogenicity assessment.

Methods in Molecular Biology 1425. (2016) 107-120. Benfenati E (Ed.). In silico Methods for Predicting Drug Toxicity. Springer, New York, USA (2016)

Golbamaki Bakhtyari A, Benfenati E, Golbamaki Bakhtyari N, Manganaro A, Merdivan E, Roncaglioni A, Gini G

New clues on carcinogenicity-related substructures derived from mining two large datasets of chemical compounds

J Environ Sci Health C Environ Carcinog Ecotoxicol Rev 2016; 34 : 97-113

Kulkarni SA, Benfenati E, Barton-Maclaren T

Improving confidence in (Q)SAR predictions under Canada's Chemicals Management Plan – a chemical space approach

SAR and QSAR in Environmental Research, 2016, 27, 851-863

Manganaro A, Pizzo F, Lombardo A, Pogliaghi A, Benfenati E

Predicting persistence in the sediment compartment with a new automatic software based on the k-Nearest Neighbor (k-NN) algorithm

Chemosphere 2016; 144 : 1624-1630,

Manganelli S, Benfenati E

Use of read-across tools.

Methods in Molecular Biology 1425. (2016) 305-324. Benfenati E (Ed.). In silico Methods for Predicting Drug Toxicity. Springer, New York, USA (2016)

Manganelli S, Leone C, Toropov AA, Toropova AP, Benfenati E

QSAR model for predicting cell viability of human embryonic kidney cells exposed to SiO2 nanoparticles

Chemosphere 2016, 144, 995-1001,

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. **(https://www.journals.elsevier.com/materials-today-proceedings)**

Manganelli S, Benfenati E, Manganaro A, Kulkarni S, Barton-Maclaren T, Honma M.

New quantitative structure–activity relationship models improve predictability of Ames mutagenicity for aromatic azo compounds. Toxicol. Sci. 2016 ; 153 : 316-326- doi:10.1093/toxsci/kfw125

Mansouri K, Abdelaziz A, Rybacka A, Roncaglioni A, Tropsha A, Varnek A, Zakharov A, Worth A, Richard AM, Grulke CM, Trisciuzzi D, Fourches D, Horvath D, Benfenati E, Muratov E, Wedebye EB, Grisoni F, Mangiatordi GF, Incisivo GM, Hong H, Ng HW, Tetko IV, Balabin I, Kancherla J, Shen J, Burton J, Nicklaus M, Cassotti M, Nikolov NG, Nicolotti O, Andersson PL, Zang Q, Politi R, Beger RD, Todeschini R, Huang R, Farag S, Rosenberg SA, Slavov S, Hu X, Judson RJ.

CERAPP: Collaborative Estrogen Receptor Activity Prediction Project

Environ Health Perspect, 2016; 124: 1023-1033. DOI: 10.1289/ehp.1510267

Marzo M, Kulkarni S, Manganaro A, Roncaglioni A, Wu S, Barton-Maclaren T S, Lester C, Benfenati E

Integrating in silico models to enhance predictivity for developmental toxicity

Toxicology 2016; 370: 127-137

Marzo M, Roncaglioni R, Kulkarni S, Barton-Maclaren TS, Benfenati E

In silico model for developmental toxicity: how to use QSAR models and interpret their results.

Methods in Molecular Biology 1425. (2016) 139-162. Benfenati E (Ed.). In silico Methods for Predicting Drug Toxicity. Springer, New York, USA

Mombelli E, Raitano G, Benfenati E

In silico prediction of chemically induced mutagenicity: how to use QSAR models and interpret their results.

Methods in Molecular Biology 1425. (2016) 87-106. Benfenati E (Ed.). In silico Methods for Predicting Drug Toxicity. Springer, New York, USA

Porta N, Roncaglioni A, Marzo M, Benfenati E

QSAR methods to screen endocrine disruptors

Nucl Receptor Res 2016. Article ID 101203, 13 pages. doi:10.11131/2016/101203

Pizzo F, Benfenati E

In silico model for repeated-dose toxicity (RTD): prediction of the noobserved adverse effect level (NOAEL) and lowest observed adverse effect level (LOAEL).

Methods in Molecular Biology 1425. (2016) 163-176. Benfenati E (Ed.). In silico Methods for Predicting Drug Toxicity. Springer, New York, USA (2016)

Pizzo F, Lombardo A, Brandt M, Manganaro A, Benfenati E

A new integrated in silico strategy for the assessment and prioritization of persistence of chemicals under REACH

Environment International, 2016, 88, 250-260

Pizzo F, Lombardo A, Manganaro A, Benfenati E

A New Structure-Activity Relationship (SAR) Model for Predicting Drug-Induced Liver Injury, Based on Statistical and Expert-Based Structural Alerts

Frontiers in Pharmacology, 2016, 7, Article 442, 15 pages, doi: 10.3389/fphar.2016.00442

Pizzo F, Lombardo A, Manganaro A, Cappelli C I, Petoumenou M I, Albanese F, Roncaglioni A, Brandt M, Benfenati E

Integrated in silico strategy for PBT assessment and prioritization under REACH

Environ Res 2016; 151: 478-492,

Toropov A A, Toropova A P, Benfenati E, Fanelli R

QSAR as a random event: Selecting of the molecular structure for potential anti-tuberculosis agents

Antiinfect Agents 2016 ; 14 : 3-10

Toropov A A, Toropova A P, Cappellini L, Benfenati E, Davoli E

Odor threshold prediction by means of the Monte Carlo method

Ecotoxicol Environ Saf 2016; 133: 390-394

Toropova A P, Toropov A A, Manganelli S, Leone C, Baderna D, Benfenati E, Fanelli R

Quasi-SMILES as a tool to utilize eclectic data for predicting the behavior of nanomaterials

NanoImpact 2016 ; 1 : 60-64

Toropova A P, Toropov A A, Veselinovic A M, Veselinovic J B, Benfenati E, Leszczynska D, Leszczynksy J

Nano-QSAR: Model of mutagenicity of fullerene as a mathematical function of different conditions

Ecotoxicol Environ Saf 2016; 124 : 32-36

2015

Baderna D, Lomazzi E, Passoni A, Pogliaghi A, Petoumenou MI, Bagnati R, Lodi M, Viarengo A, Sforzini S, Benfenati E, Fanelli R

Chemical characterization and ecotoxicity of three soil foaming agents used in mechanized tunneling

Journal of Hazardous Materials 2015, 296, 210–220

Baderna D, Lomazzi E, Pogliaghi A, Ciaccia G, Lodi M, Benfenati E.

Acute phytotoxicity of seven metals alone and in mixture: Are Italian soil threshold concentrations suitable for plant protection? Environmental Research, 2015, 140: 102-111, ISSN 0013-9351, http://dx.doi.org/10.1016/j.envres.2015.03.023.

Benfenati E, Manganelli S, Giordano S, Raitano G, Manganaro A

Hierarchical Rules for Read-Across and In Silico Models of Mutagenicity

Journal of Environmental Science and Health, Part C, 33:385–403, 2015.

Benfenati E, Roncaglioni A, Petoumenou M I, Cappelli C I, Gini G

Integrating QSAR and read-across for environmental assessment

SAR QSAR Environ Res 2015 ; 26 : 605-618

Cappelli CI, Benfenati E, Cester J

Evaluation of QSAR models for predicting the partition coefficient (log P) of chemicals under the REACH regulation

Environmental Research 2015, 143, 26–32

Cappelli CI, Cassano A, Golbamaki A, Moggio Y, Lombardo A, Colafranceschi M, Benfenati E

Assessment of in silico models for acute aquatic toxicity towards fish under REACH regulation

SAR and QSAR in Environmental Research, 2015, 26, 977-999.

Kamath P, Raitano G, Fernández A, Rallo R, Benfenati E

In silico exploratory study using structure–activity relationship models and metabolic information for prediction of mutagenicity based on the Ames test and rodent micronucleus assay

SAR and QSAR in Environmental Research, 2015, 26, 1017-1031

Fàbrega F, Kumar V, Benfenati E, Schuhmacher M, Domingo JL, Nadal M

Physiologically-based pharmacokinetic modeling of perfluoroalkyl substances in the human body

Toxicological & Environmental Chemistry 2015, 97, 814-827

DOI 10.1080/02772248.2015.1060976

Gissi A, Lombardo A, Roncaglioni A, Gadaleta D, Mangiatordi GF, Nicolotti O, Benfenati E

Evaluation and comparison of benchmark QSAR models to predict a relevant REACH endpoint: The bioconcentration factor (BCF)

Environmental Research, 2015, 137: 398–409

Golbamaki N, Rasulev B, Cassano A, Marchese Robinson RL, Benfenati E, Leszczynski J, Cronin MT.

Genotoxicity of metal oxide nanomaterials: review of recent data and discussion of possible mechanisms.

Nanoscale. 2015; 7: 2154-2198.

Gonella Diaza R, Manganelli S, Esposito A, Roncaglioni A, Manganaro A, Benfenati E

Comparison of in silico tools for evaluating rat oral acute toxicity

SAR QSAR Environ Res 2015 ; 26 : 1-27

Petoumenou M I, Pizzo F, Cester J, Fernandez A, Benfenati E

Comparison between bioconcentration factor (BCF) data provided by industry to the European Chemicals Agency (ECHA) and data derived from QSAR models

Environ Res 2015 ; 142 : 529-534 ,

Pizzo F, Gadaleta D, Lombardo A, Nicolotti O, Benfenati E

Identification of structural alerts for liver and kidney toxicity using repeated dose toxicity data

Chem Cent J 2015 ; 9 : 62.

Roncaglioni A, Benfenati E, Mantovani A, Fiorino F, Perissutti E, Lorenzetti S

The Role of In Silico Tools in Supporting the Application of the Substitution Principle

Altex, 2015, 32: 151-153.

Severino B, Fiorino F, Corvino A, Caliendo G, Santagada V, Assis D M, Oliveira J R, Juliano L, Manganelli S, Benfenati E, Frecentese F, Perissutti E, Juliano M A

Synthesis, biological evaluation and docking studies of PAR2-AP derived pseudopeptides as inhibitors of kallikrein 5 and 6

Biol Chem 2015 ; 396 : 45-52

Toropov AA, Toropova AP, Cappelli CI, Benfenati E

CORAL: Model for octanol/water partition coefficient

Fluid Phase Equilibria 2015; 397: 44–49

Toropov A A, Toropova A P, Pizzo F, Lombardo A, Gadaleta D, Benfenati E

CORAL: model for no observed adverse effect level (NOAEL)

Mol Divers 2015 ; 19 : 563-575,

Toropova A P, Toropov A A, Benfenati E

CORAL: Prediction of binding affinity and efficacy of thyroid hormone receptor ligands

Eur J Med Chem 2015 ; 101 : 452-461

Toropova A P, Toropov A A, Benfenati E,

A quasi-QSPR modelling for the photocatalytic decolourization rate constants and cellular viability (CV%) of nanoparticles by CORAL

SAR and QSAR in Environmental Research, 2015; 26: 29-40

Toropova A P, Toropov A A, Benfenati E, Korenstein R, Leszczynska D, Leszczynksy J

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 Int 2015 ; 22 : 745-757

Toropova A P, Toropov A, Benfenati E, Leszczynska D, Leszczynksy J

QSAR model as a random event: A case of rat toxicity

Bioorg Med Chem 2015 ; 23 : 1223-1230

Toropova AP, Toropov AA, Veselinovic JB, Veselinovic AM, Benfenati E, Leszczynska D, Leszczynski J

Application of the Monte Carlo Method to Prediction of Dispersibility of Graphene inVarious Solvents

Int. J. Environ. Res., 2015, 9, 1211-1216

Trisciuzzi D, Alberga D, Mansouri K, Judson R, Cellamare S, Catto M, Carotti A, Benfenati E, Novellino E, Mangiatordi GF, Nicolotti O.

Docking-based classification models for exploratory toxicology studies on high-quality estrogenic experimental data.

Future Med Chem 2015, 7, 1921-1936.

2014

Gini G, Franchi AM, Manganaro A, Golbamaki A, Benfenati E

ToxRead: A tool to assist in read across and its use to assess mutagenicity of chemicals

SAR and QSAR in Environmental Research, 2014, 25: 999-1011

Baderna D, Colombo A, Romeo M, Cambria F, Teoldi F, Lodi M, Diomede L, Benfenati E

Soil quality in the Lomellina area using in vitro models and ecotoxicological assays

Environmental Research 2014, 133:220–231

Floris M, Manganaro A, Nicolotti O, Medda R, Mangiatordi GF, Benfenati E

A generalizable definition of chemical similarity for read-across

Journal of Cheminformatics 2014, 6:39

Sforzini S, Moore M, Boeri M, Benfenati E, Colombo A, Viarengo A

Immunofluorescence detection and localization of B[a]P and TCDD in earthworm tissues

Chemosphere 2014; 107 : 282-289

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 TiO2 nanoparticles

Ecotoxicol Environ Saf 2014 ; 108 : 203-209

Gadaleta D, Pizzo F, Lombardo A, Carotti A, Escher S, Nicolotti O, Benfenati E

A k-NN algorithm for predicting the oral sub-chronic toxicity in the rat

ALTEX 2014 ; 31 : 423-432. IF 5.467

Cassano A, Raitano G, Mombelli E, Fernández A, Cester J, Roncaglioni A, Benfenati E

Evaluation of QSAR Models for the Prediction of Ames Genotoxicity: A Retrospective Exercise on the Chemical Substances Registered Under the EU REACH Regulation

Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2014, 32: 273-298

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

Struct Chem 2014 ; 25 : 1067-1073

Nicolotti O, Benfenati E, Carotti A, Gadaleta D, Gissi A, Mangiatordi GF, Novellino E

REACH and in silico methods: an attractive opportunity for medicinal chemists

Drug Discovery Today 2014, 19: 1757-1768.

Toropova A P, Toropov A A, Benfenati E, Korenstein R

QSAR model for cytotoxicity of SiO2 nanoparticles on human lung fibroblasts

J Nanopart Res 2014 ; 16 : 2282

Gissi A, Gadaleta D, Floris M, Olla S, Carotti A, Novellino E, Benfenati E, Nicolotti O

An Alternative QSAR-Based Approach for Predicting the Bioconcentration Factor for Regulatory Purposes

ALTEX, 2014, 31: 23–36

Golbamaki Bakhtyari A, Cassano Antonio, Lombardo A, Moggio Y, Colafranceschi M, Benfenati E

Comparison of in silico models for prediction of Daphnia magna acute toxicity

SAR QSAR Environ Res 2014 ; 25 : 673-694

Lombardo A, Pizzo F, Benfenati E, Manganaro A, Ferrari T, Gini G.

A new in silico classification model for ready biodegradability, based on molecular fragments

Chemosphere, 108, 2014, 10-16

Lombardo A, Roncaglioni A, Benfentati E, Nendza M, Segner H, Fernández A, Kühne R, Franco A, Pauné E, Schüürmann G. Integrated testing strategy (ITS) for bioaccumulation assessment under REACH

Environ Int. 2014 ; 69C:40-50. IF 5.559

Lombardo A, Roncaglioni A, Benfenati E, Nendza M, Segner H, Jeram S, Pauné E, Schuurmann G

Optimizing the aquatictoxicity assessment under REACH through an integrated testing strategy (ITS)

Environ Res 2014 ; 135 : 156-164

2013

Stefan Scholz, Erika Sela, Ludek Blaha, Thomas Braunbeck, Malyka Galay-Burgos, Mauricio García-Franco, Joaquin Guinea, Nils Klüver, Kristin Schirmer, Katrin Tanneberger, Marysia Tobor-Kapłon, Hilda Witters, Scott Belanger, Emilio Benfenati, Stuart Creton, Mark T.D. Cronin, Rik I.L. Eggen, Michelle Embry, Drew Ekman, Anne Gourmelon, Marlies Halder.

A European perspective on alternatives to animal testing for environmental hazard identification and risk assessment

Regulatory Toxicology and Pharmacology, 2013, 67: 506-530

Nendza M, Gabbert S, Ku¨**hne R, Lombardo A, Roncaglioni A, Benfenati E, Benigni R, Bossa C, Strempel S, Scheringer M,**

Fernández A, Rallo R, Giralt F, Dimitrov S, Mekenyan O, Bringezu F, Schu¨**u¨rmann G**

A comparative survey of chemistry-driven in silico methods to identify hazardous substances under REACH

Regulatory Toxicology and Pharmacology 2013; 66 : 301–314

Maggioni S, Balaguer P, Chiozzotto C, Benfenati E

Screening of endocrine-disrupting phenols, herbicides, steroid estrogens, and estrogenicity in drinking water from the waterworks of 35 Italian cities and from PET-bottled mineral water

Environ Sci Pollut Res Int 2013 ; 20 : 1649-1660

Roncaglioni A, Toropov AA, Toropova AP, Benfenati E

In silico methods to predict drug toxicity

Current Opinion in Pharmacology 2013, 13:1–5

Ducharme N A, Peterson L E, Benfenati E, McCollum C, Gustafsson J - A, Bondesson M

Meta-analysis of toxicity and teratogenicity of 133 chemicals from zebrafish developmental toxicity studies

Reprod Toxicol 2013 ; 41 : 98-108

Ferrari T, Cattaneo D, Gini G, Golbamaki Bakhtyari N, Manganaro A Benfenati E

Automatic knowledge extraction from chemical structures: the case of mutagenicity prediction

SAR and QSAR in Environmental Research 2013; 24 : 365-383

Golbamaki Bakhtyari N, Raitano G, Benfenati E, Martin T M, Young D

Comparison of in silico models for prediction of mutagenicity

J Environ Sci Health C Environ Carcinog Ecotoxicol Rev 2013 31 : 45-66

Baderna D, Colombo A, Amodei G, Cantù S, Teoldi F, Cambria F, Rotella G, Natolino F, Lodi M, Benfenati E

Chemical-based risk assessment and in vitro models of human health effects induced by organic pollutants in soils from the Olona valley

Science of the Total Environment 2013; 463-464 : 790–801

Benfenati E, Pardoe S, Martin T M, Gonella Diaza R, Lombardo A, Manganaro A, Gissi A

Using toxicological evidence from QSAR models in practice

Altex 2013 30 : 19-40

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

Boriani E, Benfenati E, Baderna D, Thomsen M

Application of ERICA index to evaluation of soil ecosystem health according to sustainability threshold for chemical impact

Science of the Total Environment 2013 443 : 134-142

Cappelli C I, Manganelli S, Lombardo A, Gissi A, Benfenati E

Validation of quantitative structure-activity relationships models to predict water-solubility of organic compounds

Science of the Total Environment 2013, 463-464: 781–789

Pizzo F, Lombardo A, Manganaro A, Benfenati E

In silico models for predicting ready biodegradability under REACH: a comparative study

Science of the Total Environment 2013, 463–464: 161–168

Toropova A P, Toropov A A, Martyanov S E, Benfenati E, Gini G, Leszczynska D, Leszczynski J

CORAL: Monte Carlo method as a tool for the prediction of the bioconcentration factor of industrial pollutants

Mol Inform 2013 32 : 145-154

Gissi A, Nicolotti O, Carotti A, Gadaleta D, Lombardo A, Benfenati E

Integration of QSAR models for bioconcentration suitable for REACH

Science of the Total Environment 2013 ; 456-457 : 325–332

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

Toropov AA, Toropova AP, Benfenati E, Gini G.

OCWLGI Descriptors: Theory and Praxis

Current Computer-Aided Drug Design 2013; 9: 226-232

Vigh E, Colombo A, Benfenati E, Hakansson H, Berglund M, Bódis J, Garai J

Individual breast milk consumption and exposure to PCBs and PCDD/Fs in Hungarian infants: A time-course analysis of the first three months of lactation

Science of the Total Environment 2013; 449 : 336-344

Toropova AP, Toropov AP, Puzyn T, Benfenati E, Leszczynska D, Leszczynski D

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

Colombo A, Benfenati E, Bugatti S G, Lodi M, Mariani A, Musmeci L, Rotella G, Senese V, Ziemacki G, Fanelli R

PCDD/Fs and PCBs in ambient air in a highly industrialized city in Northern Italy

Chemosphere 2013; 90 : 2352-2357

Toropov A A, Toropova A P, Benfenati E, Gini G, Leszczynska D, Leszczynski J

CORAL: QSPR model of water solubility based on local and global SMILES attributes

Chemosphere 2013, 90 : 877-880

Kohonen P, Benfenati E, Bower D, Ceder R, Crump M, Cross K, Grafstrom R C, Healey L, Helma C, Jeliazkova N, Maggioni S, Miller S, Myatt G, Rautenberg M, Stacey G, Willighagen E, Wiseman J, Hardy B

The ToxBank data warehouse: Supporting the replacement of in vivo repeated dose systemic toxicity testing

Molecular Informatics 2013, 32 : 47-63

Toropova A P, Toropov A A, Benfenati E, Gini G, Leszczynska D, Leszczynski J

CORAL: QSPRs of enthalpies of formation of organometallic compounds

J Math Chem 2013; 51: 1684-1693

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

Cent Eur J Chem 2013 11 : 371-380

Maggioni S, Bagnati R, Pandelova M, Schramm K W, Benfenati E

Genistein and dicarboximide fungicides in infant formulae from the EU market

Food Chemistry 2013 136 : 116-119

2012

Toropov A A, Toropova A P, Benfenati E, Gini G, Leszczynska D, Leszczynski J

CORAL: Classification model for predictions of anti-sarcoma activity

Curr Top Med Chem 2012 12 : 2741-2744

Toropov A A, Toropova A P, 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 2012 ; 23 : 1891-1904

Toropov A A, Toropova A P, Rasulev B, Benfenati E, Gini G, Leszczynska D, Leszczynski J

CORAL: Binary classifications (active/inactive) for liver-related adverse effects of drugs

Current Drug Safety 2012 7 : 257-261

Toropov AA, Toropova AP, Benfenati E, Gini G, Fanelli R

The definition of the molecular structure for potential anti-malaria agents by the Monte Carlo method.

Struct Chem 2013; 24:1369–1381

Toropova A P, Toropov A A, Benfenati E, Gini G, Leszczynska D, Leszczynski J

CORAL: Models of toxicity of binary mixtures

Chemometrics Intelligent Laboratory System 2012 119 : 39-43

Mays C, Benfenati E, Pardoe S

Use and perceived benefits and barriers of QSAR models for REACH: findings from a questionnaire to stakeholders

Chem Cent J 2012 6 : 159

Toropova A P, Toropov A A, 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 2012 ; 23 : 1873-1878

Toropov A A, Toropova A P, Benfenati E, Gini G, Puzyn T, Leszczynska D, Leszczynski J

Novel application of the CORAL software to model cytotoxicity of metal oxide nanoparticles to bacteria Escherichia coli

Chemosphere 2012 89 : 1098-1102

Toropova A P, Toropov A A, Benfenati E, Gini G, Leszczynska D, Leszczynski J

CORAL: Quantitative models for estimating bioconcentration factor of organic compounds

Chemometrics Intelligent Laboratory System 2012 118 : 70-73

Toropov A A, Toropova A P, Benfenati E, Gini G, Leszczynska D, Leszczynski J

Calculation of molecular features with apparent impact on both activity of mutagens and activity of anticancer agents

Anticancer Agents Med Chem 2012 : 12 807-817

Fernández A, Lombardo A, Rallo R, Roncaglioni A, Benfenati E, Giralt F

Quantitative consensus of bioaccumulation models for integrated testing strategies

Environ Int 2012 45 : 51-58. IF 6.248

Toropova A P, Toropov A A, Benfenati E, Gini G, Leszczynska D, Leszczynski J

The minimum number of "eccentric" substances: quantitative criterion to estimate the reliability of a QSPR. A case of water solubility

Chem Phys Lett 2012 542 : 134-137

Toropov A A, Toropova A P, Rasulev B, Benfenati E, Gini G, Leszczynska D, Leszczynski J

CORAL: QSPR modeling of rate constants of reactions between organic aromatic pollutants and hydroxyl radical

J Comput Chem 2012 33 : 1902-1906

Toropov A A, Toropova A P, Lombardo A, Roncaglioni A, De Brita N, Stella G, Benfenati E

CORAL: the prediction of biodegradation of organic compounds with optimal SMILES-based descriptors

Cent Eur J Chem 2012 10 : 1042-1048

Toropova A P, Toropov A A, Lombardo A, Roncaglioni A, Benfenati E, Gini G

CORAL: QSAR models for acute toxicity in Fathead minnow (Pimephales Promelas)

J Comput Chem 2012 33 : 1218-1223

Toropova A P, Toropov A A, 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 2012 79 : 332-338

Toropov A A, Toropova A P, Gonella Diaza R, Benfenati E, Gini G

SMILES-based optimal descriptors: QSAR modeling of estrogen receptor binding affinity by correlation balance

Struct Chem 2012 23 : 529-544

Toropova AP, Toropov AA, Benfenati E, Gini G, Leszczynska D, Leszczynski J

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 2012 ; 542 : 134-137

Toropov A A, Toropova A P, Martyanov S E, Benfenati E, Gini G, Leszczynska D, Leszczynski 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 2012 112 : 65-70

Toropova A P, Toropov A A, Martyanov S E, Benfenati E, Gini G, Leszczynska D, Leszczynski J

CORAL: QSAR modeling of toxicity of organic chemicals towards Daphnia magna

Chemometrics Intelligent Laboratory System 2012 110 : 177-181

2011

Fjodorova N, Novich M, Roncaglioni A, Benfenati E

Evaluating the applicability domain in the case of classification predictive models for carcinogenicity based on the counter propagation artificial neural network

J Comput Aid Mol Des 2011 25 : 1147-1158

Milan C, Schifanella O, Roncaglioni A, Benfenati E

Comparison and possible use of in silico tools for carcinogenicity within REACH legislation

J Environ Sci Health C 2011 29 : 300-323 IF 5.16

Benfenati E, Gonella Diaza R, Cassano Antonio, Pardoe S, Gini G, Mays C, Knauf R, Benighaus L

The acceptance of in silico models for REACH: Requirements, barriers, and perspectives

Chem Cent J 2011 5 : 58

Toropov A A, Toropova A P, Benfenati E, Gini G, Leszczynska D, Leszczynski J

SMILES-based QSAR approaches for carcinogenicity and anticancer activity: Comparison of correlation weights for identical SMILES attributes

Anti-Cancer Agents in Medicinal Chemistry 2011 11 : 974-982

Toropov A A, Toropova A P, Martyanov S E, Benfenati E, Gini G, Leszczynska D, Leszczynski J

Comparison of SMILES and molecular graphs as the representation of the molecular structure for QSAR analysis for mutagenic potential of polyaromatic amines

Chemometrics Intelligent Laboratory System 2011 109 : 94-100

Colombo A, Benfenati E, Bugatti S G, Celeste G, Lodi M, Rotella G, Senese V, Fanelli R

Concentrations of PCDD/PCDF in soil close to a secondary aluminum smelte

Chemosphere 2011 85 : 1719-1724

Casalegno M, Benfenati E, Sello G

Identification of toxifying and detoxifying moieties for mutagenicity prediction by priority assessment

J Chem Inf Model 2011 51 : 1564-1574

Toropova A P, Toropov A A, Benfenati E, Gini G, Leszczynska D, Leszczynski J

CORAL: Quantitative Structure–Activity Relationship models for estimating toxicity of organic compounds in rats

J Comput Chem 2011 42 : 2727-2733

Toropova A P, Toropov A A, Benfenati E, Gini G, Leszczynska D, Leszczynksi J

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 2011 9 : 846-854

Bilitewski B, Barcelo D, Darbra R M, v.d. Voet E, Belhaj M, Benfenati E, Grundmann V

Report on the 1st workshop of the RISKCYCLE coordination action. Hanoi, Vietnam, 4–5 May 2010

Environ Sci Pollut Res 2011 18 : 827-828

Adler S, Basketter D, Creton S, Pelkonen O, Van Benthem J, Zuang V, Andersen K E, Angers-Loustau A, Aptula A O, Bal-Price A, Benfenati E, Bernauer U, Bessems J, Bois F Y, Boobis A, Brandon E, Bremer S, Broschard T, Casati S, Coecke S, Corvi R, Cronin M T D, Daston G, Dekant W, Felter S, Grignard E, Gundert-Remy U, Heinonen T, Kimber I, Kleinjans J, Komulainen H, Kreiling R, Kreysa J, Leite S B, Loizou G, Maxwell G, Mazzatorta P, Munn S, Pfuhler S, Phrakonkham P, Piersma A, Poth A, Prieto P, Repetto G, Rogiers V, Schoeters G, Schwarz M, Serafimova R, Tahti H, Testai E, Van Delft J, van Loveren H, Vinken M, Worth A, Zaldivar J

Alternative (non-animal) methods for cosmetics testing: current status and future prospects-2010

Arch Toxicol 2011 85 : 367-485

Toropova A P, Toropov A A, Benfenati E, Gini G

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 2011 77 : 343-360

Toropova A P, Toropov A A, Benfenati E, Gini G, Leszczynska D, Leszczynksi J

CORAL: Quantitative Structure–Activity Relationship models for estimating toxicity of organic compounds in rats

J Comput Chem 2011 42 : 2727-2733

Baderna D, Maggioni S, Boriani E, Gemma S, Molteni M, Lombardo A, Colombo A, Bordonali S, Rotella G, Lodi M, Benfenati E

A combined approach to investigate the toxicity of an industrial landfill's leachate: chemical analyses, risk assessment and in vitro assays

Environmental Research 2011 111 : 603-613

Toropova A P, Toropov A A, Benfenati E, Gini G, Leszczynska D, Leszczynksy J

CORAL: QSPR models for solubility of [C60] and [C70] fullerene derivatives

Mol Divers 2011 15 : 249-256

Benfenati E, Toropov A A, Toropova A P, Manganaro A, Gonella Diaza R

CORAL Software: QSAR for Anticancer Agents

Chem Biol Drug Des 2011 77 : 471-476

Toropov A A, Toropova A P, Lombardo A, Roncaglioni A, Benfenati E, Gini G

CORAL: Building up the model for bioconcentration factor and defining it's applicability domain

Eur J Med Chem 2011 46 : 1400-1403

Toropova A P, Toropov A A, Benfenati E, Gini G

Co-evolutions of correlations for QSAR of toxicity of organometallic and inorganic substances: An unexpected good prediction based on a model that seems untrustworthy

Chemometrics Intelligent Laboratory System 2011 105 : 215-219

Toropova A P, Toropov A A, Gonella Diaza R, Benfenati E, Gini G

Analysis of the co-evolutions of correlations as a tool for QSAR-modeling of carcinogenicity: an unexpected good prediction based on a model that seems untrustworthy

Cent Eur J Chem 2011 9 : 166-174

Toropova A P, Toropov A A, Benfenati E, Gini G

QSAR modelling toxicity toward rats of inorganic substances by means of CORAL

Cent Eur J Chem 2011 9 : 75-85

2010

Toropova A P, Toropov A A, Benfenati E, Leszczynska D, Leszczynksi J

QSAR modeling of measured binding affinity for fullerene-based HIV-1 PR inhibitors by CORAL

J Math Chem 2010 48 : 959-987

Benfenati E, Gini G, Hoffman S, Luttik R

Comparing in vivo, in vitro and in silico methods and integrated strategies for chemical assessment: problems and prospects

Altern Lab Anim 2010 38 : 153-166

Piir G, Sild S, Roncaglioni A, Benfenati E, Maran U

QSAR model for the prediction of bio-concentration factor using aqueous solubility as the main descriptor

SAR QSAR Environ Res 2010 21 : 711-729

Viganò L, Benfenati E, Bottero S, Cevasco A, Monteverde M, Mandich A

Endocrine modulation, inhibition of ovarian development and hepatic alterations in rainbow trout exposed to polluted river water

Environmental Pollution 2010 158 : 3675-3683

Cassano A, Manganaro A, Martin T M, Young D, Piclin N, Pintore M, Bigoni D, Benfenati E

The CAESAR models for developmental toxicity

Chem Cent J 2010 4 (Suppl 1) : S4

Fjodorova N, Vrachko M, Novich M, Roncaglioni A, Benfenati E

New public QSAR model for carcinogenicity

Chem Cent J 2010 4 (Suppl 1) : S3

Lombardo A, Roncaglioni A, Boriani E, Milan C, Benfenati E

Assessment and validation of the CAESAR predictive model for bioconcentration factor (BCF) in fish

Chem Cent J 2010 4 (Suppl 1) : S1

Benfenati E

The CAESAR Project for in silico models for the REACH legislation

Chem Cent J 2010 4 (Suppl 1) : I1

Lombardo A, Gonella Diaza R, Roncaglioni A, Benfenati E

CAESAR's approach for alternative in silico methods for REACH

Altex 2010 27 : 109-116

Toropov A A, Toropova A P, Benfenati E

SMILES-based optimal descriptors: QSAR modeling of carcinogenicity by balance of correlations with ideal slopes

Eur J Med Chem 2010 45 : 3581-3587

Toropova A P, Toropov A A, Lombardo A, Roncaglioni A, Benfenati E, Gini G

A new bioconcentration factor model based on SMILES and indices of presence of atoms

Eur J Med Chem 2010 45 : 4399-4402

Boriani E, Mariani A, Baderna D, Moretti C, Lodi M, Benfenati E

ERICA: a multiparametric toxicological risk index for the assessment of environmental healthiness

Environment International 2010 36 : 665-674

Senese V, Boriani E, Baderna D, Mariani A, Lodi M, Finizio A, Testa S, Benfenati E

Assessing the Environmental Risks Associated with Contaminated Sites: definition of an ecotoxicological classification index for landfill areas (ECRIS)

Chemosphere 2010 80 : 60-66

Toropov A A, Toropova A P, Benfenati E, Leszczynska D, Leszczynksi J

InChI-based optimal descriptors: QSAR analysis of fullerene[C60]-based HIV-1 PR inhibitors by correlation balance

Eur J Med Chem 2010 45 : 1387-1394

Toropov A A, Toropova A P, Raska I, Benfenati E

QSPR modeling of octanol/water partition coefficient of antineoplastic agents by balance of correlations

Eur J Med Chem 2010 45 : 1639-1647

Toropov A A, Toropova A P, Benfenati E, Leszczynska D, Leszczynksi J

Use of the international chemical identifier for constructing QSPR-model of normal boiling points of acyclic carbonyl substances

J Math Chem 2010 47 : 355-369

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 2010 14 : 183-192

Toropov A A, Toropova A P, Benfenati E, Leszczynska D, Leszczynksy J

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 2010 47: 647-666

Toropov A A, Toropova A P, Benfenati E, Leszczynska D, Leszczynksy J

SMILES-based optimal descriptors: QSAR modeling of fullerene-based HIV-1 PR inhibitors by balance of correlations with ideal slopes

J Comput Chem 2010 31 : 381-392

Toropov A A, Toropova A P, Benfenati E, Manganaro A

QSAR modelling of the toxicity to Tetrahymena pyriformis by balance of correlations

Mol Divers 2010 14 : 821-827

Toropov AA, Toropova AP, Benfenati E

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 2010; 8 : 1047-1052

2009

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

Toropov A A, Toropova A P, Benfenati E, Manganaro A

QSAR modelling of carcinogenicity by balance of correlations

Mol Divers 2009 13 : 367-373

Toropov A A, Toropova A P, Benfenati E

QSPR modelling of the octanol/water partition coefficient of organometallic substances by optimal SMILES-based descriptors

Cent Eur J Chem 2009 7 : 846-856

Toropov A A, Toropova A P, Benfenati E, Leszczynska D, Leszczynksy J

Additive InChI-based optimal descriptors: QSPR modeling of fullerene C60 solubility in organic solvents

J Mat Chem 2009 46 : 1232-1251

Toropov A A, Toropova A P, Benfenati E

Additive SMILES-based carcinogenicity models: Probabilistic principles in the search for robust prediction

Int J Mol Sci 2009 10 : 3106-3127

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 2009 46 : 1060-1073

Toropov A A, Toropova A P, Benfenati E, Manganaro A

QSPR modeling of enthalpies of formation for organometallic compounds by SMART-based optimal descriptors

J Comput Chem 2009 30 : 2576-2582

Toropov A A, Toropova A P, Benfenati E

QSPR modeling bioconcentration factor (BCF) by balance of correlations

Eur J Med Chem 2009 44 : 2544-2551

Benfenati E, Benigni R, DeMarini D M, Helma C, Kirkland D, Martin T M, Mazzatorta P, Ouédraogo-Arras G, Richard A M, Schilter B, Schoonen W G E J, Snyder R D, Yang C

Predictive Models for Carcinogenicity and Mutagenicity: Frameworks, State-of-the-Art, and Perspectives

J Environ Sci Health C 2009 27 : 57-90

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

Chem Biol Drug Des 2009 73 : 515-525

Maggioni S, Benfenati E, Colosio C, Moretto A, Roots O, Tasiopoulou S, Visentin S

Food contamination control in European new member states and associated candidate countries: data collected within the SAFEFOODNET project

J Environ Sci Health B 2009 44: 407-414

Toropov A A, Toropova A P, Benfenati E

QSAR Modelling for Mutagenic Potency of Heteroaromatic Amines by Optimal SMILES-based Descriptors

Chemical Biology and Drug Design 2009 73 : 301-312

Colombo A, Benfenati E, Mariani G, Lodi M, Marras R, Rotella G, Senese V, Fattore E, Fanelli R

PCDD/Fs in ambient air in north-east Italy: the role of a MSWI inside an industrial area

Chemosphere 2009 77 : 1224-1229

2008

Roncaglioni A, Piclin N, Pintore M, Benfenati E

Binary classification models as screening tools for endocrine disrupter effects mediated through the estrogen receptor

SAR QSAR Environ Res 2008 19 : 697-733

Viganò L, Benfenati E, van Cauwenberge A, Eidem J K, Erratico C, Goksøyr A, Kloas W, Maggioni S, Mandich A, Urbatzka R

Estrogenicity profile and estrogenic compounds determined in river sediments by chemical analysis, ELISA and yeast assays

Chemosphere 2008 73 : 1078-1089

Casalegno M, Sello G, Benfenati E

Definition and detection of outliers in chemical space

J Chem Inf Model 2008 48 : 1592-1601

Zhao C, Boriani E, Chana A, Roncaglioni A, Benfenati E

A new hybrid QSAR model for the prediction of bioconcentration factors (BCF)

Chemosphere 2008 73 : 1701-1707

Toropov A A, Toropova A P, Benfenati E

QSPR modeling for enthalpies of formation of organometallic compounds by means of SMILES-based optimal descriptors

Chemical Physics Letters 2008 461 : 343-347

Slavov S, Gini G, Benfenati E

QSAR trout toxicity models on aromatic pesticides

J Environ Sci Health B 2008 43 : 633-637

Colombo A, Benfenati E, Karelson M, Maran U

Definition of a univocal architecture for chemical splitting to optimise QSAR models for aquatic toxicity

Chemosphere 2008 72 : 772-780

Fjodorova N, Novic M, Vracko M, Smirnov V, Kharchevnikova N, Zholdakova Z, Novikov S, Skvortsova N, Filimonov D, Poroikov V, Benfenati E

Directions in QSAR Modeling for Regulatory Uses in OECD Member Countries, EU and in Russia

J Environ Sci Health C 2008 26 : 201-236

Toropov A A, Benfenati E

Additive SMILES-based optimal descriptors in QSAR modelling bee toxicity: Using rare SMILES attributes to define the applicability domain

Bioorg Med Chem 2008 16 : 4801-4809

Bursztyka J, Perdu E, Tulliez J, Debrauwer L, Delous G, Canlet C, De Sousa G, Rahmani R, Benfenati E, Cravedi J-P

Comparison of genistein metabolism in rats and humans using liver microsomes and hepatocytes

Food Chem Toxicol 2008 46: 939-948

Porcelli C, Roncaglioni A, Chana A, Benfenati E

A comparison of DEMETRA individual QSARs with an index with an index of evaluation of uncertainty

Chemosphere 2008 71: 1845-1852.

Fjororova N, Novich M, Vrachko M, Kharchevnichova N, Zholdakova Z, Sinitzyna O, Benfenati E

Regulatory assessment of chemicals within OECD Member Countries, EU and in Russia

J Environ Sci Health C 2008 26: 40-88

Roncaglioni A, Benfenati E

In silico-aided prediction of biological properties of chemicals: oestrogen receptor-mediated effects

Chem Soc Rev 2008 37: 441-450 IF 17.419

Porcelli C, Boriani E, Roncaglioni A, Chana A, Benfenati E

Regulatory perspectives in the use and validation of QSAR. A case study: DEMETRA model for daphnia toxicity

Environ Sci Technol 2008 42 : 491-496

Pandelova M, Henkelmann B, Roots O, Simm M, Jarv L, Benfenati E, Schramm K-W

Levels of PCDD/F and dioxin-like PCB in Baltin fish of different age and gender

Chemosphere 2008 71: 369-378

2007

Gini G, Benfenati E

E-modelling: foundations and cases for applying AI to life sciences

International Journal on Artificial Intelligence Tools 2007 16 2 : 243-268

Boriani E, Spreafico M, Benfenati E, Novic M

Structural features of diverse ligands influencing binding affinities to estrogen alpha and estrogen beta receptors. Part I: molecular descriptors calculated from minimal energy conformation of isolated ligands.

Mol Divers 2007 11: 153-169.

Boriani E, Spreafico M, Benfenati E, Novic M

Structural features of diverse ligands influencing binding affinities to estrogen alpha and estrogen beta receptors. Part II. Molecular descriptors calculated from conformation of the ligands in the complex resulting from previous docking study

Mol Divers 2007 11: 171-181.

Benfenati E

Predicting toxicity through computers: a changing world

Chemistry Central Journal 2007 1: 32

Toropov A A, Benfenati E

SMILES in QSPR/QSAR modeling: Results and perspectives

Current Drug Discovery Technologies 2007 4 : 77-116

Benigni R, Netzeva T, Benfenati E, Bossa C, Franke R, Helma C, Hulzebos E, Marchant C, Richard A, Woo Y-T, Yang C

The expanding role of predictive toxicology: An update on the (Q)SAR models for mutagens and carcinogens

J Environ Sci Health C 2007 25 : 53-97

Mandich A, Bottero S, Benfenati E, Cevasco A, Erratico C, Maggioni S, Massari A, Pedemonte F, Viganò L

In vivo exposure of carp to graded concentrations of bisphenol A

Gen Comp Endocr 2007 153 : 15-24

Benfenati E

The specificity of the QSAR models for regulatory purposes: the example of the DEMETRA project

SAR QSAR Environ Res 2007 18 : 209-220

Maran U, Sild S, Mazzatorta P, Casalegno M, Benfenati E, Romberg M

Grid computing for the estimation of toxicity: Acute toxicity on fathead minnow (Pimephales promelas)

Lect Notes Comput Sci 2007 4360 : 60-74

Urbatzka R, van Cauwenberge A, Maggioni S, Viganò L, Mandich A, Benfenati E, Lutz I, Kloas W

Androgenic and antiandrogenic activities in water and sediment samples from the river Lambro, Italy, detected by yeast androgen screen and chemical analyses

Chemosphere 2007 67 : 1080-1087

Fratev F, Lo Piparo E, Benfenati E, Mihaylova E

Toxicity study of allelochemical-like pesticides by combination of 3DQSAR, docking, local binding energy (LBE) and GRID approaches

SAR QSAR Environ Res 2007 18 : 675-692

Toropov A A, Benfenati E

Optimisation of correlation weights of SMILES invariants for modelling oral quail toxicity

Eur J Med Chem 2007 42 : 606-613

Kahn I, Maran U, Benfenati E, Netzeva T I, Schultz T W, Cronin M T D

Comparative quantitative structure-activity-activity relationships for toxicity to Tetrahymena pyriformis and Pimephales promelas

Altern Lab Anim 2007 35 : 15-24

Toropov A A, Benfenati E

SMILES as an alternative to the graph in QSAR modelling of bee toxicity

Comput Biol Chem 2007 31 : 57-60

2006

Calliera M, Finizio A, Azimonti G, Benfenati E, Trevisan M

Harmonised pesticide risk trend indicator for food (HAPERITIF): the methodological approach

Pest Manag Sci 2006 62 : 1168-1176

Vracko M, Brandelj V, Barbieri P, Benfenati E, Chaudhry Q, Cronin M, Devillers J, Gallegos A, Gini G, Gramatica P, Helma C, Neagu D, Netzeva T, Pavan M, Patlevicz G, Randic M, Tsakovska I, Worth A

Validation of counter propagation neural network models for predictive toxicology according to the OECD principles. A case study

SAR QSAR Environ Res 2006 17 : 265-284

Casalegno M, Benfenati E, Sello G

Application of a fragment-based model to the prediction of the genotoxicity of aromatic amines

Internet Electronic Journal Molecular Design 2006 5: 431-446

Lo Piparo E, Koehler K, Chana A, Benfenati E

Virtual screening for aryl hydrocarbon receptor binding prediction

J Med Chem 2006 49 : 5702-5709

Tolfsen CC, Sundback LV, Softeland T, Urbatzka R, Vigano L, Kloas W, Mandich A, Benfenati E, Goksoyr A, Grosvik BE

Proteome studies of carp and frog exposed endocrine disrupting compounds

Marine Environmental Research 2006, 62: S159-S159

Mazzatorta P, Cronin M T D, Benfenati E

A QSAR study of avian oral toxicity using support vector machines and genetic algorithms

QSAR Combinatorial Science 2006 25 : 616-628

Casalegno M, Sello G, Benfenati E

Top-priority fragment QSAR approach in predicting pesticide aquatic toxicity

Chem Res Toxicol 2006 19 : 1533-1539

Duchowicz P R, Castro E A, Toropov A A, Benfenati E

Application of flexible molecular descriptors in the QSPR-QSAR study of heterocyclic drugs

Topics Heterocyclic Chemistry 2006 3 : 1-38

Lemke F, Benfenati E, Mueller J A

Data-driven modeling and prediction of acute toxicity of pesticide residues

SIGKDD Explorations 2006 8 : 71-79

Lo Piparo E, Fratev F, Lemke F, Mazzatorta P, Smiesko M, Fritz J I, Benfenati E

QSAR models for Daphnia magna toxicity prediction of benzoxazinone allelochemicals and their transformation products

J Agric Food Chem 2006 54 : 1111-1115

Lo Piparo E, Smiesko M, Mazzatorta P, Benfenati E, Idinger J, Blumel S

Preliminary analysis of toxicity of benzoxazinones and their metabolites for Folsomia candida

J Agric Food Chem 2006 54 : 1099-1104

Toropov A A, Benfenati E

QSAR models for Daphnia toxicity of pesticides based on combinations of topological parameters of molecular structures

Bioorg Med Chem 2006 14 : 2779-2788

Toropov A A, Benfenati E

QSAR models of quail dietary toxicity based on the graph of atomic orbitals

Bioorg Med Chem 2006 16 : 1941-1943

Viganò L, Mandich A, Benfenati E, Bertolotti R, Bottero S, Porazzi E, Agradi E

Investigating the estrogenic risk along the River Po and its intermediate section

Arch Environ Contam Toxicol 2006 51 : 641-651

Piclin N, Pintore M, Wechman C, Roncaglioni A, Benfenati E, Chretien J R

Ecotoxicity prediction by adaptive fuzzy partioning. Comparing descriptors computed on 2D and 3D structures

SAR QSAR Environ Res 2006 17 : 225-251

Toropov A A, Benfenati E

Correlation weighting of valence shells in QSAR analysis of toxicity

Bioorg Med Chem 2006 14 : 3923-3928

2005

Fratev F, Benfenati E,

3D-QSAR and molecular mechanics study for the differences in the azole activity against yeastlike and filamentous fungi and their relation to P450DM inhibition. 1. 3-substituted-4(3H)-quinazolinones

J Chem Inf Model 2005 45 : 634-644

Mandich A, Benfenati E, Cronin MTD, Goksøyr A, Grøsvik BE, Kloas W, Van Cauwenberge A, Viganò L

Environmental Agent Susceptibility Assessment Using Existing and Novel Biomarkers as Rapid Noninvasive Testing Methods

Ann NY Acad Sci 2005 1040 : 381-386

Mazzatorta P, Smiesko M, Lo Piparo E, Benfenati E

QSAR model for predicting pesticide aquatic toxicity

J Chem Inf Model 2005 45 : 1767-1774

Kovatcheva A, Cronin M T D, Benfenati E, Roncaglioni A, Lo Piparo E

Identification of the structural requirements of the receptor-binding affinity of diphenolic azoles to estrogen receptors alpha and beta by three-dimensional quantitative structure-activity relationship and structure-activity relationship analysis

J Med Chem 2005 48 : 7628-7636

Smiesko M, Benfenati E

Thermodynamic descriptors derived from density functional theory calculations in prediction of aquatic toxicity

J Chem Inf Model 2005 45 : 379-385

Casalegno M, Benfenati E, Sello G

An automated group contribution method in predicting aquatic toxicity: The diatomic fragment approach

Chem Res Toxicol 2005 18 : 740-746

Porazzi E, Pardo Martinez M, Fanelli R, Benfenati E

GC-MS analysis of dichlobenil and its metabolites in groundwater

Talanta 2005 68 : 146-154

Sild S, Maran U, Romberg M, Schuller B, Benfenati E

Open MolGRID: Using automated workflows in GRID computing environment

Lect Notes Comput Sci 2005 3470 : 464-473

Netzeva T I, Aptula A O, Benfenati E, Cronin M T D, Gini G, Lessigiarska I, Maran U, Vracko M, Schuurmann G

Description of the electronic structure of organic chemicals using semiempirical and ab initio methods for development of toxicological QSARs

J Chem Inf Model 2005 45 : 106-114

Pierucci P, Porazzi E, Pardo Martinez M, Adani F, Carati C, Rubino F M, Colombi A, Calcaterra E, Benfenati E

Volatile organic compounds produced during the aerobic biological processing of municipal solid waste in a pilot plant

Chemosphere 2005 59 : 423-430

2004

Roncaglioni A, Benfenati E, Boriani E, Clook M

A protocol to select high quality datasets of ecotoxicity values for pesticides

J Environ Sci Health B 2004 B39 : 641-652

Smiesko M, Benfenati E

Predictive models for aquatic toxicity of aldehydes designed for various model chemistries

J Chem Inf Comput Sci 2004 44 : 976-984

Gini G, Craciun M, Koenig C, Benfenati E

Combining unsupervised and supervised artificial neural networks to predict aquatic toxicity

J Chem Inf Comput Sci 2004 44 : 1897-1902

Benfenati E, Mariani G, Lodi M, Reitano G, Fanelli R

Is bioexsiccation releasing dioxins?

Organohalogen Compounds 2004 66 : 955-961

Roncaglioni A, Novic M, Vracko M, Benfenati E

Classification of potential endocrine disrupters on the basis of molecular structure using a nonlinear modeling method

J Chem Inf Comput Sci 2004 44 : 300-309

Toropov A A, Benfenati E

QSAR modelling of aldehyde toxicity against a protozoan, Tetrahymena pyriformis by optimization of correlation weights of nearest neighboring codes

Journal Molecular Structure (Theochem) 2004 679 : 225-228

Toropov A A, Benfenati E

QSAR modelling of aldehyde toxicity by means of optimisation of correlation weights of nearest neighbouring codes

Journal Molecular Structure (Theochem) 2004 676 : 165-169

Mazzatorta P, Benfenati E, Lorenzini P, Vighi M

QSAR in ecotoxicity: An overview of modern classification techniques

J Chem Inf Comput Sci 2004 44 : 105-112

Koenig C, Gini G, Craciun M, Benfenati E

Multiclass classifier from a combination of local experts: Toward distributed computation for real-problem classifiers

International Journal Pattern Recognition Artificial Intelligence 2004 18 : 801-817

2003

Mazzatorta P, Vracko M, Benfenati E

ANVAS: Artificial neural variables adaptation system for descriptor selection

J Comput Aid Mol Des 2003 17 : 335-346

Benfenati E, Barceló D, Johnson I, Galassi S, Levsen K

Emerging organic contaminants in leachates from industrial waste landfills and industrial effluent

Trends Analytical Chemistry 2003 22 : 757-765

Pintore M, Piclin N, Benfenati E, Gini G, Chretien J R

Predicting toxicity against the fathead minnow by adaptive fuzzy partition

QSAR Combinatorial Science 2003 22 : 210-219

Benfenati E, Porazzi E, Bagnati R, Forner F, Pardo Martinez M, Mariani G, Fanelli R

Organic tracers identification as a convenient strategy in industrial landfills monitoring

Chemosphere 2003 51 : 677-683

Mazzatorta P, Vracko M, Jezierska A, Benfenati E

Modeling toxicity by using supervised Kohonen neural networks

J Chem Inf Comput Sci 2003 43 : 485-492

Pintore M, Piclin N, Benfenati E, Gini G, Chretien J R

Database mining with adaptive fuzzy partition: Application to the prediction of pesticide toxicity on rats

Environ Toxicol Chem 2003 22 : 983-991

Mazzatorta P, Benfenati E, Neagu C D, Gini G

Tuning neural and fuzzy-neural networks for toxicity modeling

J Chem Inf Comput Sci 2003 43 : 513-518

Fattore E, Di Guardo A, Mariani G, Guzzi A, Benfenati E, Fanelli R

Polychlorinated dibenzo-p-dioxin and dibenzofurans in the air of Seveso, Italy, 26 years after the explosion

Environmental Science Technology 2003 37 : 1503-1508

Benfenati E, Gini G, Piclin N, Roncaglioni A, Vari M R

Predicting logP of pesticides using different software

Chemosphere 2003 53 : 1155-1164

2002

Mazzatorta P, Benfenati E, Neagu C D, Gini G

The importance of scaling in data mining for toxicity prediction

J Chem Inf Comput Sci 2002 42 : 1250-1255

Tavazzi S, Benfenati E, Barceló D

Accelerated solvent extraction then liquid chromatography coupled with mass spectrometry for determination of 4-t-octylphenol, 4-nonylphenols, and biphenol A in fish liver

Chromatographia 2002 56 : 463-467

Benfenati E, Genah D, Verro R, Mazzatorta P

Chemical analysis, distributed modelling and risk indices. Three fundamentals pillars in risk assessment

Scientific World Journal 2002 2 : 1617-1625

Mariani G, Carasi S, Fattore E, Nichetti S, Guzzi A, Benfenati E, Fanelli R

Fast and simple method for PCB analysis in human serum samples by GC-NICI-MS

Organohalogen Compounds 2002 55 : 111-114

Fattore E, Viganò L, Mariani G, Guzzi A, Benfenati E, Fanelli R

Polychlorinated dibenzo-p-dioxins and dibenzofurans in river Po sediments

Chemosphere 2002 49 : 749-754

Krikunova V, Hegedus G, My Le H, Jouravleva L, Eremin S, Natangelo M, Benfenati E, Szekacs A

Development of an enzyme-linked immunosorbent assay (ELISA) for the herbicide propanil

Int J Environ Anal Chem 2002 82 : 865-878

Natangelo M, Tavazzi S, Benfenati E

Evaluation of solid phase microextraction-gas chromatography in the analysis of some pesticides with different mass spectrometric techniques: Application to environmental waters and food samples

Anal Lett 2002 35 : 327-338

2001

Fattore E, Viganò L, Mariani G, Guzzi A, Benfenati E, Fanelli R

Polychlorinated dibenzo-p-dioxins (PCDDs) and furans (PCDFs) in the river Po sediments

Organohalogen Compounds 2001 51 : 53-57

Benfenati E, Piclin N, Roncaglioni A, Vari M R

Factors influencing predictive models for toxicology

SAR QSAR Environ Res 2001 12 : 593-603

Sello G, Sala L, Benfenati E

Predicting toxicity: A mechanism of action model of chemical mutagenicity

Mutat Res Fundam Mol Mech Mutag 2001 479 : 141-171

Krasnova A, Eremin S, Natangelo M, Tavazzi S, Benfenati E

A polarization fluorescence immunoassay for the herbicide propanil

Anal Lett 2001 34 : 2285-2301

Katritzky A R, Petrukhin R, Tatham D, Basak S, Benfenati E, Karelson M, Maran U

Interpretation of quantitative structure - property and - activity relationships

J Chem Inf Comput Sci 2001 41 : 679-685

2000

Galassi S, Benfenati E

Fractionation and toxicity evaluation of waste waters

J Chromatogr A 2000 889 : 149-154

1999

Gini G, Lorenzini M, Benfenati E, Grasso P, Bruschi M

Predictive carcinogenicity: A model for aromatic compounds, with nitrogen-containing substituents, based on molecular descriptors using an artificial neural network

J Chem Inf Comput Sci 1999 39 : 1076-1080

Natangelo M, Tavazzi S, Fanelli R, Benfenati E

Analysis of some pesticides in water samples using solid-phage microextraction-gas chromatography with different mass spectrometric techniques

J Chromatogr A 1999 859 : 193-201

Benfenati E, Pierucci P, Fanelli R, Preiss A, Godejohann M, Astratov M, Levsen K, Barceló D

Comparative studies of the leachate of an industrial landfill by gas chromatography-mass spectrometry, liquid chromatography-nucelar magnetic resonance and liquid chromatography-mass spectrometry

J Chromatogr A 1999 831 : 243-256

Natangelo M, Mangiapan S, Bagnati R, Benfenati E, Fanelli R

Increased concentrations of nitrophenols in leaves from a damaged forestal site

Chemosphere 1999 38 : 1495-1503

1998

Grasso P, Benfenati E, Terreni M, Pregnolato M, Natangelo M, Pagani G

Deuterated internal standards for gas chromatographic-mass spectrometric analysis of polar organophosphorus pesticides in water samples

J Chromatogr A 1998 822 : 91-99

Gini G, Testaguzza V, Benfenati E, Todeschini R

Hybrid toxicology expert system: Architecture and implementation of a multi-domain hybrid expert system for toxicology

Chemometrics Intelligent Laboratory System 1998 43 : 135-145

Fattore E, Mueller L, Davoli E, Castelli D, Benfenati E

Industrial pollutants in ground waters from Northern Milan

Chemosphere 1998 36 : 2007-2017

Benfenati E, Grasso P, Molina C, Barceló D, Giarei C, Galassi S, Guzzella L, Grabec Svegl I, Stella G, Ogorevc B

An interlaboratory analysis on labile pesticides

Toxicological Environmental Chemistry 1998 65 : 173-184

Benfenati E, Pierucci P, Niego D

A case study of indoor pollution by Chinese cooking

Toxicological Environmental Chemistry 1998 65 : 217-224

1997

Mangiapan S, Benfenati E, Grasso P, Terreni M, Pregnolato M, Pagani G, Barceló D

Metabolites of alachlor in water: Identification by mass spectrometry and chemical synthesis

Environmental Science Technology 1997 31 : 3637-3646

Fattore E, Benfenati E, Mariani G, Cools E, Vezzoli G, Fanelli R

Analysis of organic micropollutants in sediment samples of the Venice Lagoon, Italy

Water Air Soil Pollut 1997 99 : 237-244

Mueller L, Fattore E, Benfenati E

Determination of aromatic amines by solid-phase microextraction and gas chromatography-mass spectrometry in water samples

J Chromatogr A 1997 791 : 221-230

Fattore E, Benfenati E, Mariani G, Fanelli R, Evers E H G

Patterns and sources of polychlorinated dibenzo-p-dioxins and dibenzofurans in sediments from the Venice Lagoon, Italy

Environmental Science Technology 1997 31 : 1777-1784

Benfenati E, Gini G

Computational predictive programs (expert systems) in toxicology

Toxicology 1997 119 : 213-225

1996

Fattore E, Benfenati E, Marelli R, Cools E, Fanelli R

Sterols in sediment samples from Venice lagoon, Italy

Chemosphere 1996 33 : 2383-2393

Molina C, Grasso P, Benfenati E, Barceló D

Determination and stability of phenmediphan, ethofumesate and fenamiphos in ground water samples using automated solid phase extraction cartridges followed by liquid chromatography high flow pneumatically assisted electrospray mass spectrometry

Int J Environ Anal Chem 1996 65 : 69-82

Benfenati E, Facchini G, Pierucci P, Fanelli R

Identification of organic contaminants in leachates from industrial waste landfills

Trends Analytical Chemistry 1996 15 : 305-310

Grabec I, Ogorevc B, Novic M, Benfenati E

Solid-phase extraction coupled with electrochemical detection for the determination of the herbicide bromofenoxim in water samples at low- and sub-ug I-1 levels

Analyst 1996 121 : 1839-1843

Terreni M, Benfenati E, Pregnolato M, Bellini A, Giavini D, Bavetta S F, Molina C, Barceló D

Synthesis and use of deuterated fenamiphos and its metabolites as internal standards for mass spectrometric analysis in water

J Chromatogr A 1996 754 : 207-219

Galassi S, Provini A, Mangiapan S, Benfenati E

Alachlor and its metabolites in surface water

Chemosphere 1996 32 : 229-237

Fattore E, Benfenati E, Fanelli R

Analysis of chlorinated 1,3-butadienes by solid-phase microextraction and gas chromatography-mass spectrometry

J Chromatogr A 1996 737 : 85-91

Hassan A A M, Benfenati E, Facchini G, Fanelli R

Pollution of ground and drinking water with volatile organic compounds: Solid-phase microextraction and GC/MS analysis

Toxicological Environmental Chemistry 1996 55 : 73-81

Molina C, Grasso P, Benfenati E, Barceló D

Automated sample preparation with extraction columns followed by liquid chromatography-ionspray mass

spectrometry. Interferences, determination and degradation of polar organophosphorus pesticides in water samples

J Chromatogr A 1996 737 : 47-58

Hassan A A M, Benfenati E, Fanelli R

Detection and quantitation of trihalomethanes in drinking water from Alexandria, Egypt

Bull Environ Contam Toxicol 1996 56 : 397-404

Benfenati E, Terreni M, Facchini G, Grasso P, Fanelli R

Analysis of pesticides and related products by chromatography-mss spectrometry. Development of a project of the European Community

Journal Analytical Chemistry (Transl Zh Anal Khim) 1996 51 : 1091-1094

1995

Terreni M, Pregnolato M, Resnati G, Benfenati E

Selective sulfur oxygenation in phosphoroamidate, thionophosphate, and thiophosphate agrochemicals by perfluoro-cis-2,3-dialkyloxaziridine

Tetrahedron 1995 51 : 7981-7992

Cai X, Ogorevc B, Benfenati E, Kalcher K, Novic M, Grabec I

Batch square-wave voltammetric and flow-injection amperometric determination of trace amounts of bromofenoxim

Anal Chim Acta 1995 310 : 153-160

Benfenati E, Terreni M, Rovida C, Stella G

Analysis of bromofenoxim by supercritical fluid chromatography and comparison with an HPLC method

Toxicological Environmental Chemistry 1995 47 : 119-128

Magistrelli A, Villa P, Benfenati E, Modest E J, Salmona M, Tacconi M T

Fate of 1-O-octadecyl-2-O- methyl-rac- glycero- 3-phosphocholine (ET18-OMe) in malignant cells, normal cells, and isolated and perfused rat liver

Drug Metab Dispos 1995 23 : 113-118

Natangelo M, Romagnano S, Guzzella L, Benfenati E

GC analysis of some organochlorine pesticides using a brominated internal standard

Int J Environ Anal Chem 1995 58 : 55-66

Terreni M, Benfenati E, Pistotti V, Fanelli R

A library report on the analysis of pesticides subject to investigation for the European Communities Commission

Int J Environ Anal Chem 1995 58 : 31-42

Benfenati E, Garofani S, Natangelo M, Mangiapan S, Fanelli R

Impurities released from extractive phases used in the analysis of pesticides

Int J Environ Anal Chem 1995 58 : 23-30

Mariani G, Benfenati E, Fanelli R

A NICI-GC-MS method to analyze endosulfan in biological samples

Int J Environ Anal Chem 1995 58 : 67-72

1994

Bussolino F, Arese M, Silvestro L, Soldi R, Benfenati E, Sanavio F, Aglietta M, Bosia A, Camussi G

Involvement of a serine protease in the synthesis of platelet-activating factor by endothelial cells stimulated by tumor necrosis factor-alpha or interleukin-1alpha

Eur J Immunol 1994 24 : 3131-3139

Terreni M, Benfenati E, Natangelo M, Facchini G, Pagani G

Synthesis and use of pentadeuteriumethyl ethofumesate as an internal standard for the determination of ethofumesate and its metabolites in water by gas chromatography-mass spectrometry

J Chromatogr A 1994 688 : 243-250

Benfenati E, Cools E, Fattore E, Fanelli R

A GC-MS method for the analysis of fecal and plant sterols in sediment samples

Chemosphere 1994 29 : 1393-1405

Benfenati E, Mariani G, Schiavon G, Lodi M, Fanelli R

Diurnal, weekly and seasonal air concentrations of PCDD and PCDF in an industrial area

Fresenius Journal Analytical Chemistry 1994 348 : 141-143

Benfenati E, Frassanito R, Di Toro N, Fanelli R, Brandt A, Di Rella M, Cecchetelli L

Mass spectrometric studies of flavonoids

Natural Product Letters 1994 4 : 247-254

Frassanito R, Benfenati E, Ciotti G, Fanelli R

A simple method for determination of N-nitrosamine traces in trifluralin samples by gas chromatography-mass spectrometry

Toxicological Environmental Chemistry 1994 45 : 199-204

1993

Noris M, Benigni A, Boccardo P, Gotti E, Benfenati E, Aiello S, Todeschini M, Remuzzi G

Urinary excretion of platelet activating factor in patients with immunemediated glomerulonephritis

Kidney Int 1993 43 : 426-429

Natangelo M, Benfenati E, De Gregorio G, Fanelli R, Ciotti G

GC-MS analysis of n-phosphonomethyl-glycine (glyphosate) samples through derivatization with a perfluoroanhydride and trifluoroethanol: Identification of by-products

Toxicological Environmental Chemistry 1993 38 : 225-232

Garattini S, Mariani G, Benfenati E, Fanelli R

Preliminary survey on 2,3,7,8-TCDD in cellulose- containing consumer products on the Italian market

Chemosphere 1993 27 : 1561-1564

1992

Benfenati E, Di Toro N, Fanelli R, Lualdi G, Tridico R, Stella G, Buscaini P, Stimilli L

Characterization of organic and inorganic pollutants in the Adige river (Italy)

Chemosphere 1992 25 : 1665-1674

Mariani G, Benfenati E, Fanelli R, Nicoli A, Bonfitto E, Jacopone S

Incineration of agro-industrial wastes and macro- and micropollutants emission

Chemosphere 1992 24 : 1545-1551

Benfenati E, Perico N, Peterlongo F, Imberti O, Schieppati A, Remuzzi G

Analysis by fast atom bombardment mass spectrometry of phospholipids from tubuli, glomeruli, and urine of normal rats and rats with acute renal failure

Biochem Med Metab Biol 1992 48 : 219-226

Benfenati E, Natangelo M, Fanelli R, Lualdi G, Tridico R

Quantification of 4,4'-diaminodiphenylmethane by gas chromatography negative ion chemical ionization mass spectrometry

Microchemical Journal 1992 46 : 352-359

Benfenati E, Valzacchi S, Mariani G, Airoldi L, Fanelli R

PCDD, PCDF, PCB, PAH, cadmium and lead in roadside soil: Relationship between road distance and concentration

Chemosphere 1992 24 : 1077-1083

Benfenati E, Natangelo M, Pallucca E, Tridico R, Borghetti E, Lualdi G

Specific gas chromatography-mass spectrometry analytical method for the determination of cyhexatin in animal feed

J Chromatogr 1992 605 : 129-133

Meli G, Bagnati R, Fanelli R, Benfenati E, Airoldi L

Metabolic profile of atrazine and N-nitrosoatrazine in rat urine

Bull Environ Contam Toxicol 1992 48 : 701-708

Benfenati E, Fanelli R, Bosone E, Caponi R, Farina P

Mass spectrometric identification of urinary and plasma metabolites of 2-(6'-carboxyhexyl)-3-n-hexylcyclohexylamine, a new antiaggregating agent

Eur J Drug Metab Pharmacokinet 1992 17 : 93-101

1991

Benfenati E, Mariani G, Fanelli R, Farneti A

Synthesis and destruction of PCDD and PCDF inside a municipal solid waste incinerator

Chemosphere 1991 23 : 715-722

Benfenati E, Mariani G, Fanelli R, Zuccotti S

'De Novo' synthesis of PCDD, PCDF, PCB, PCN and PAH in a pilot incinerator

Chemosphere 1991 22 : 1045-1052

Bussolino F, Sordano C, Benfenati E, Bozzaro S

Dictyostelium cells produce platelet-activating factor in response to cyclic AMP

Eur J Biochem 1991 196 : 609-615

Celardo A, Dell'Elba G, Frassanito R, Benfenati E, Bonati M

Simultaneous determination of isbufylline and its major metabolites in rabbit blood and urine by reversed-phase high-performance liquid chromatography

J Chromatogr 1991 568 : 407-418

Benfenati E, Fanelli R, Bosone E, Biffi C, Caponi R, Cianetti M, Farina P

Mass spectrometric identification of urinary and plasma metabolites of 6-(6'-carboxyhexyl) -7-n-hexyl-1,3-diazaspiro-[4-4]-nonan-2,4-dione, a new cytoprotective agent

Drug Metab Dispos 1991 19 : 913-916

Natangelo M, Bagnati R, Fanelli R, Gavinelli M, Ulbricht C, Benfenati E

Preparation of 4,4'-diaminodiphenylmethane-(2H4) for use as internal standard in quantification of 4,4'-

diaminodiphenylmethane

Journal Labelled Compounds Radiopharmaceuticals 1991 29 : 725-728

Macconi D, Noris M, Benfenati E, Quaglia P, Pagliarino G, Remuzzi G

Increased urinary excretion of platelet activating factor in mice with lupus nephritis

Life Sci 1991 48 : 1429-1437

Benfenati E, Natangelo M, Davoli E, Fanelli R

Migration of vinyl chloride into PVC-bottled drinking-water assessed by gas chromatography-mass spectrometry

Food Chem Toxicol 1991 29 : 131-134

1990

Bagnati R, Benfenati E, Mariani G, Fanelli R, Chiesa G, Moro G, Pitea D

The combustion of municipal solid waste and PCDD and PCDF emissions. On the real scale thermal behavior of PCDD and PCDF in flue gas and fly ash

Chemosphere 1990 20 : 1907-1914

Benfenati E, Tremolada P, Chiappetta L, Frassanito R, Bassi G, Di Toro N, Fanelli R, Stella G

Simultaneous analysis of 50 pesticides in water samples by solid phase extraction and GC-MS

Chemosphere 1990 21 : 1411-1421

Chen S, Kirschner G, Benfenati E

Quantitative analysis of 1-stearoyl-2-oleoyl-sn -glycero-3-phosphoserine by negative-ion fast-atom bombardment mass spectrometry

Rapid Commun Mass Spectrom 1990 4 : 214-216

Mariani G, Benfenati E, Fanelli R

Concentrations of PCDD and PCDF in different points of a modern refuse incinerator

Chemosphere 1990 21 : 507-517

Benfenati E, Icardi G, Chen S, Fanelli R

Syntheses of deuterated leu-enkephalins and their use as internal standards for quantification of leu-enkephalin by fast atom bombardment mass spectrometry

Journal Labelled Compounds Radiopharmaceuticals 1990 28 : 411-419

1989

Benfenati E, De Bellis G, Chen S, Bettazzoli L, Fanelli R, Tacconi M T, Kirschner G, Pege G

A fast atom bombardment-mass spectrometric method to quantitate lysophosphatidylserine in rat brain

J Lipid Res 1989 30 : 1983-1986

Benfenati E, Macconi D, Noris M, Icardi G, Bettazzoli L, De Bellis G, Gavinelli M, Rotondo S, Remuzzi G

Development of a mass spectrometric method to quantitate platelet activating factor in mouse urine

J Lipid Res 1989 30 : 1977-1981

Celardo A, Bortolotti A, Benfenati E, Bonati M

Measurement of vitamin E in premature infants by reversed-phase high-performance liquid chromatography

J Chromatogr 1989 490 : 432-438

Rotondo S, Zucchetti M, Sessa C, D'Incalci M, Benfenati E, Fanelli R

A gas chromatographic mass spectrometric assay for the determination of aphidicolin in plasma of cancer patients

J Pharm Sci 1989 78 : 399-401

Chen S, Benfenati E, Fanelli R, Kirschner G, Pregnolato F

Molecular species analysis of phospholipids by negative ion fast atom bombardment mass spectrometry: Application of surface precipitation technique

Biomed Environ Mass Spectrom 1989 18 : 1051-1056

Benfenati E, Zucchetti M, D'Incalci M

Identification of microsomal metabolites of spirogermanium

Anticancer Res 1989 9 : 507-510

Benfenati E, Farina P, Colombo T, De Bellis G, Capodiferro M V, D'Incalci M

Metabolism and pharmacokinetics of p-(3,3- dimethyl-1-triazeno) benzoic acid in M5076 sarcoma-bearing mice

Cancer Chemother Pharmacol 1989 24 : 354-358

1988

Candiano G, Ghiggeri G M, Gusmano R, Zetta L, Benfenati E, Icardi G

Reaction of 2-amino-2-deoxy-D-glucose and lysine: Isolation and characterization of 2,5-

Carbohydr Res 1988 184 : 67-75

Bagnati R, Benfenati E, Davoli E, Fanelli R

Screening of 21 pesticides in water by single extraction with C18 silica bonded phase columns and HRGC-MS

Chemosphere 1988 17 : 59-65

Benfenati E, Fanelli R, Chiabrando C, Valcavi U, Bosone E, Farina P

Mass spectrometric identification of urinary and plasma metabolites of 9-hydroxy-19,20 -bis-nor-prostanoic acid (Rosaprostol)

Prostaglandins 1988 35 : 665-684

Arigoni R, Chiste R, Makovec F, Setnikar I, Benfenati E, Fanelli R

Identification of metabolites of tiropramide in human urine

Biomed Environ Mass Spectrom 1988 15 : 205-209

Latini R, Sica A, Marchi S, Chen Z M, Gavinelli M, Benfenati E

High-performance liquid chromatographic separation and mass spectrometric identification of propafenone, 5-hydroxypropafenone and N-depropylpropafenone

J Chromatogr 1988 424 : 211-214

Pastorelli R, Ancidei A, Benfenati E, Fanelli R, Airoldi L

Effect of butylated hydroxyanisole added in vitro or administered to rats on N,N-dibutylnitrosamine and N-butyl-N-(4-hydroxybutyl)nitrosamine metabolism by hepatic S9 preparations

Toxicology 1988 48 : 71-80

1987

Davoli E, Benfenati E, Bagnati R, Fanelli R

Analysis of atrazine in underground waters at part per trillion levels as an early warning method for contamination and for soil distribution studies

Chemosphere 1987 16 : 1425-1430

Benfenati E, Caccia S, Della Vedova F

1-(o-Methoxyphenyl)-piperazine is a metabolite of drugs bearing a methoxyphenylpiperazine side-chain

J Pharm Pharmacol 1987 39 : 312-313

1996

Benfenati E, Pastorelli R, Castelli M G, Fanelli R, Carminati A, Farneti A, Lodi M

Studies on the tetrachlorodibenzo-p-dioxins (TCDD) and tetrachlorodibenzofurans (TCDF) emitted from an urban incinerator

Chemosphere 1986 15 : 557-561

1985

Farina P, Benfenati E, Lassiani L, Nisi C, D'Incalci M

High-performance liquid chromatographic assay for the determination of p-(3,3-dimethyl-1-triazeno)benzoic acid in mouse plasma

J Chromatogr 1985 345 : 323-331

Broggini M, Rossi C, Benfenati E, D'Incalci M, Fanelli R, Gariboldi P

Horseradish peroxidase/hydrogen peroxide-catalyzed oxidation of VP16-213. Identification of a new metabolite

Chem Biol Interact 1985 55 : 215-224

Benfenati E, Reginato R

A comparison of three methods of soft ionization mass spectrometry of crude phospholipid extracts

Biomed Environ Mass Spectrom 1985 12 : 643-651

Colombo T, D'Incalci M, Donelli M G, Bartosek I, Benfenati E, Farina P, Guaitani A

Metabolic studies of a podophyllotoxin derivative (VP16) in the isolated perfused liver

Xenobiotica 1985 15 : 343-350

1984

Castelli M G, Benfenati E, Pastorelli R, Salmona M, Fanelli R

Kinetics of 3-tert-butyl-4-hydroxyanisole (BHA) in man

Food Chem Toxicol 1984 22 : 901-904

Airoldi L, Bonfanti M, Fanelli R, Bove B, Benfenati E, Gariboldi P

Identification of a nitrosamino aldehyde and a nitrosamino acid resulting from beta-oxidation of N-

Chem Biol Interact 1984 51 : 103-113

Caccia S, Notarnicola A, Fong M H, Benfenati E

Identification and quantitation of 1-aryl-piperazines, metabolites of drugs containing an aryl-piperazine side-chain, in rat plasma and brain

J Chromatogr 1984 283 : 211-221

Bonati M, Gaspari F, D'Aranno V, Benfenati E, Neyroz P, Galletti F, Tognoni G

Physicochemical and analytical characteristics of amiodarone

J Pharm Sci 1984 73 : 829-831

1983

Rizzardini M, Romano M, Tursi F, Salmona M, Vecchi A, Sironi M, Gizzi F, Benfenati E, Garattini S, Fanelli R

Toxicological evaluation of urban waste incinerator emissions

Chemosphere 1983 12 : 559-564

Fong M H, Abbiati A, Benfenati E, Caccia S

Quantitative analysis of minaprine and some of its metabolites with application to kinetic studies in rats

J Chromatogr 1983 259 : 141-149

Farina P, Benfenati E, Reginato R, Torti L, D'Incalci M, Threadgill M D, Gescher A

Metabolism of the anticancer agent 1-(4-acetylphenyl)- 3,3-dimethyltriazene

Biomed Environ Mass Spectrom 1983 10 : 485-488

Airoldi L, Bonfanti M, Benfenati E, Tavecchia P, Fanelli R

Identification of an acidic metabolite of n-nitrosodiethanolamine isolated from rat urine

Biomed Environ Mass Spectrom 1983 10 : 334-337

Benfenati E, Gizzi F, Reginato R, Fanelli R, Lodi M, Tagliaferri R

PCDD and PCDF in emissions from an urban incinerator. 2. Correlation between concentration of micropollutants and combustion conditions

Chemosphere 1983 12 : 1151-1157

1982

Gizzi F, Reginato R, Benfenati E, Fanelli R

Polychlorinated dibenzo-p-dioxins (PCDD) and polychlorinated dibenzofurans (PCDF) in emissions from an urban incinerator. 1. Average and peak values

Chemosphere 1982 11 : 577-583

Book's chapters:

Benfenati E, Selvestrel G, Lombardo A, Luciani D

Computational Toxicological Aspects in Drug Design and Discovery, Screening Adverse Effects

In: Current Trends in Computational Modeling for Drug Discovery. S. Kar and J. Leszczynski. Springer, Cham, Switzerland, pp 213-238 (2023)

Gini G, Hung C, Benfenati E

Big data and deep learning: extracting and revisiting chemical knowledge from data

In: Big Data Analytics in Chnoinformatics and Bioinformatics. S. Basak and M. Vracko, Eds. Elsevier, Amsterdam (Netherlands) pp 115-150 (2023)

Luciani D, Colombo E, Lombardo A, Benfenati E

Towards models for bioaccumulation suitable for the pharmaceutical domain

In: Cheminformatics, QSAR and Machine Learning Applications for Novel Drug Development. K. Roy Ed. Elsevier, Amsterdam (Netherlands) pp 441-456 (2023)

Benfenati E, Lombardo A, Drgan V, Novic M, Manganaro A

The tools for aquatic toxicology within the VEGAHUB system

In: Chemometrics and Chemoinformatics in Aquatic Toxicology. K. Roy. Ed. Wiley, Hoboken NJ (USA) pp 493-512 (2022)

Blazquez M, Andreu-Sanchez O, Ballesteros A, Fernandez-Cruz ML, Gomez-Ganau CS, Gozalbes R, Hernandez-Moreno D, de Julian-Ortiz JV, Lombardo A, Marzo M, Ranero I, Riuz-Costa N, Tarazona-Diez JV, Benfenati E

Computational tools for the assessment and substitution of biocidal active substances of ecotoxicological concern: the LIFE_COMBASE project

In: Chemometrics and Chemoinformatics in Aquatic Toxicology. K. Roy. Ed. Wiley, Hoboken NJ (USA) pp 525-546 (2022)

Gini G, Benfenati E.

From data to models: mining experimental values with machine learning tools

In: Chemometrics and Chemoinformatics in Aquatic Toxicology. K. Roy. Ed. Wiley, Hoboken NJ (USA) pp 89-125 (2022)

Gómez-Ganau S, Marzo M, Gozalbes R, Benfenati E. (2020) Computational approaches to evaluate ecotoxicity of biocides: cases from the Project COMBASE. In: Ecotoxicological QSARs, Part of the Methods in Pharmacology and Toxicology book series (MIPT), Springer Protocols, Editor Kunal Roy, pages 387-404.

Benfenati E., Lombardo A. (2020) VEGAHUB for Ecotoxicological QSAR Modeling. In: Ecotoxicological QSARs, Part of the Methods in Pharmacology and Toxicology book series (MIPT), Springer Protocols, Editor Kunal Roy, pages 759-787.

Benfenati E, Roncaglioni A, Lombardo A, Manganaro A.

Integrating QSAR, Read-Across and Screening Tools: The VEGAHUB Platform as an Example.

In: Advances in Computational Toxicology:Methodologies and Applications in Regulatory Science, Hong H, Ed. Springer Nature, 2019. pp 365-382.

Maiorana S, Teoldi F, Silvani S, Mancini A, Sanguineti A, Dupin D, Sanvito T, Bonfanti A, Baderna D, Benfenati E

Is "green" braking possible? Comparative assessment of microparticles generated by traditional and innovative braking systems

In: L'ecotossicologia come strumento di gestione degli ambienti acquatici e terrestri. Atti delle giornate di studio. 8a ed. Livorno, 26-28 nov. 2018

ISPRA-Istituto Superiore Sanità Protezione e Ricerca Ambientale, Roma 2019

Benfenati E, Lombardo A, Roncaglioni A

Computational toxicology and REACH

In: Computational toxicology: risk assessment for chemicals, 1st. ed.

John Wiley & Sons, Oxford 2018

Toropova A P, Toropov A A, Benfenati E, Rallo R, Leszczynska D, Leszczynksy J

Development of Monte Carlo approaches in support of environmental research

In: Advances in QSAR modeling

Springer, Switzerland 2017

Toropov AA, Toropova AA, Benfenati E, Nicolotti O, Carotti A, Nesmerak K, Veselinovic, AM, Veselinovic JB, Duchowicz PR, Bacelo D, Castro EA, Rasulev BF, Leszczynzka D, Leszczynski J

QSPR/QSAR analyses by means of of the CORAL software

In: K. Roy (ed). Quantitative Structure-Activity Relationships in Drug Desing, Predictive Toxicology, and Risk Assessment. IGI Global. (2015) 560-585.

Baderna D, Golbamaki Bakhtyari N, Maggioni S, Vaccari M, Colacci A, Benfenati E

Toxicological characterization of waste-related products using alternative methods: three case studies

In: B. Bilitewski et al. (eds.), Global risk-based management of chemical additives II: Risk-Based assessment and management strategies, DOI 10.1007/698_2012_193, Springer-Verlag, Berlin, Germany (2012), 171-205

Golbamaki Bakhtyari N, Baderna D, Boriani E, Schuhmacher M, Heise S, Benfenati E

Toxicological and ecotoxicological studies for additives

In: B. Bilitewski et al. (eds.), Global risk-based management of chemical additives II: Risk-Based assessment and management strategies, DOI 10.1007/698_2012_193, Springer-Verlag, Berlin, Germany (2012), 73-89

Baderna D, Boriani E, Dalla Giovanna F, Benfenati E

Lubricants and additives: A point of view

In: Bilitewski B, Darbra R M, Barcelo D (Eds.), Global risk-based management of chemical additives I: Production, usage and environmental occurrence, Springer-Verlag, Berlin, Germany (2012), 109-132

Gonella Diaza R, Roncaglioni A, Benfenati E

In silico approaches to screen dietary endocrine disruptors

in: Pongratz I, Vikstrom Bergander L (Eds.), Hormone-disruptive chemical contaminants in food, Royal Society of Chemistry, Cambridge (2011), 170-183

Nendza M, Aldenberg T, Benfenati E, Benigni R, Cronin M T D, Escher S, Fernández A, Gabbert S, Giralt F, Hewitt M, Hrovat M, Jeram S, Kroese D, Madden J C, Mangelsdorf I, Rallo R, Roncaglioni A, Rorije E, Segner H, Simon-Hettich B, Vermeire T

Data quality assessment for in silico methods: A survey of approaches and needs

In: Cronin M T D, Madden J C (Eds.), In Silico toxicology: Principles and applications, Royal Society of Chemistry, Cambridge (2010), 59-117

Bala P, Ostropytskyy V , Baldridge K, Rasch K, Benfenati E, Sild S, Casalegno M, Schone R, Maran U, Schuller B, Miroslaw L, Williams N

UNICORE: A Middleware for Life Sciences Grids

in: Cannataro M (Ed.), Handbook of Research on Computational Grid Technologies for Life Sciences, Biomedicine, and Healthcare, Vol. 1, Information Science Reference (2009), 615-643

Roncaglioni A, Benfenati E

Computer-aided methodologies to predict endocrine-disrupting potency of chemicals

in: Shaw I (Ed.), CRC Press, Boca Raton (2009), 306-321

Benfenati E, Maggioni S, Campagnola G, Senese V, Lodi M, Testa S, Schramm K-W

A protocol to evaluate organic compounds present in a landfill

in: Velinni A A (Ed.), Landfill Research Trends, Nova Science Publishers (2007), 141-166

Benfenati E, Azimonti G, Auteri D, Lodi M

Environmental and ecological toxicology: Computational risk assessment

in: Ekins S (Ed.), Computational Toxicology: Risk Assessment for Pharmaceutical and Environmental Chemicals, John Wiley & Sons Inc., Hoboken NJ, USA (2007), 625-650

Benfenati E, Craciun M, Neagu C D

The use of the DEMETRA models

in: Benfenati E (Ed.), Quantitative Structure-Activity Relationships (QSAR) for Pesticide Regulatory Purposes, Elsevier Science Ltd, Amsterdam, The Netherlands (2007), 303-313

Benfenati E

The quality criteria of the DEMETRA models for regulatory purposes: Specificity, general lessons and future perspectives

in: Benfenati E (Ed.), Quantitative Structure-Activity Relationships (QSAR) for Pesticide Regulatory Purposes, Elsevier Science Ltd, Amsterdam, The Netherlands (2007), 283-301

Amaury N, Benfenati E, Boriani E, Casalegno M, Chana A, Chaudhry Q, Chretien J R, Cotterill J, Lemke F, Piclin N, Pintore M, Porcelli C, Price N, Roncaglioni A, Toropov A A

Results of DEMETRA models

in: Benfenati E (Ed.), Quantitative Structure-Activity Relationships (QSAR) for Pesticide Regulatory Purposes, Elsevier Science Ltd, Amsterdam, The Netherlands (2007), 201-281

Benfenati E, Chretien J R, Gini G, Piclin N, Pintore M, Roncaglioni A

Validation of the models

in: Benfenati E (Ed.), Quantitative Structure-Activity Relationships (QSAR) for Pesticide Regulatory Purposes, Elsevier Science Ltd, Amsterdam, The Netherlands (2007), 185-199

Amaury N, Benfenati E, Bumbaru S, Chana A, Craciun M, Chretien J R, Gini G, Guo G, Lemke F, Minzu V, Mueller J A, Neagu C D, Pintore M, Stroia S A, Trundle P

Hybrid systems

in: Benfenati E (Ed.), Quantitative Structure-Activity Relationships (QSAR) for Pesticide Regulatory Purposes, Elsevier Science Ltd, Amsterdam, The Netherlands (2007), 149-183

Benfenati E, Casalegno M, Cotterill J, Price N, Spreafico M, Toropov A A

Characterization of chemical structures

in: Benfenati E (Ed.), Quantitative Structure-Activity Relationships (QSAR) for Pesticide Regulatory Purposes, Elsevier Science Ltd, Amsterdam, The Netherlands (2007), 83-109

Benfenati E, Boriani E, Craciun M, Malazizi L, Neagu C D, Roncaglioni A

Databases for pesticide ecotoxicity

in: Benfenati E (Ed.), Quantitative Structure-Activity Relationships (QSAR) for Pesticide Regulatory Purposes, Elsevier Science Ltd, Amsterdam, The Netherlands (2007), 59-81

Benfenati E, Clook M, Friday S, Hart A

QSARs for regulatory purposes: the case for pesticide authorization

in: Benfenati E (Ed.), Quantitative Structure-Activity Relationships (QSAR) for Pesticide Regulatory Purposes, Elsevier Science Ltd, Amsterdam, The Netherlands (2007), 1-57

Lo Piparo E, Mazzatorta P, Benfenati E

Computational methods to study properties of allelochemicals and modelling of molecular interactions in allelopathy

in: Roshchina V V, Narwal S S (Eds.), Plant Cell Diagnostics - Images, Biophysical and Biochemical Processes in Allelopathy, Science Publishers, Enfield NH, USA (2007), 169-183

Lo Piparo E, Fratev F, Mazzatorta P, Smiesko M, Benfenati E

Toxicity in allelopathy: in silico approach

in: Reigosa M J, Pedrol N, Gonzalez L (Eds.), Allelopathy: A physiological process with ecological implications, Springer-Verlag, Amsterdam (2006), 105-126

Benfenati E, Porazzi E, Pardo Martinez M

Organic contaminants in leachates from industrial waste landfills

in: Barceló D (Ed.), Emerging Organic Pollutants in Waste Waters and Sludge, vol. 1 (The Handbook of Environmental Chemistry, vol. 5), Springer-Verlag GmbH, Berlin, Germany (2004), 71-97

Di Guardo A, Calamari D, Benfenati E, Halling-Sorensen B, Zuccato E, Fanelli R

Pharmaceuticals as environmental contaminants: Modelling distribution and fate

in: Kuemmerer K (Ed.), Pharmaceuticals in the Environment - Sources, Fate, Effects and Risks, Springer-Verlag GmbH, Berlin, Germany (2001), 91-102

Benfenati E, Natangelo M, Tavazzi S

Gas chromatography/mass spectrometry methods in pesticide analysis

in: Encyclopedia of Analytical Chemistry, John Wiley & Sons Ltd, Chichester (2000), 6176-6201

Benfenati E, Mueller L, Perani L, Pierucci P

Analysis of industrial pollutants in environmental samples

in: Pawliszyn J (Ed.), Applications of Solid Phase Microextraction, The Royal Society of Chemistry, Cambridge, UK (1999), 333-345

Benfenati E, Barceló D, Helweg A, Galassi S, Stella G, Levsen K, Rindone B, Balinova A

Analysis of pesticides and their degradation products: An integrated study

in: Barceló D, Angeletti G, Amanatidis G (Eds.), EC DG XII - Water Pollution Research Report 31 -

Environmental Analysis of Pesticides and Their Conversion Products in the Aquatic Environment, Comm. of the European Communities, Luxembourg (1995), 5-7

Galassi S, Provini A, De Paolis A, Benfenati E, Mangiapan S

Metabolism of alachlor and metolachlor in water

in: Barceló D, Angeletti G, Amanatidis G (Eds.), EC DG XII - Water Pollution Research Report 31 -

Environmental Analysis of Pesticides and Their Conversion Products in the Aquatic Environment, Comm. of the European Communities, Luxembourg (1995), 13-16

Benfenati E, Garofani S, Facchini G, Cantù A, Terreni M

Analysis of surface waters with different extractive procedures

in: Wrobel L C, Brebbia C A (Eds.), Water pollution II - Modelling, Measuring and Prediction, Comput. Mech. Publ. & Elsevier, Southampton, UK (1993), 341-348

Proceedings:

Dorne JL, Amzal B, Quignot N, Wiecek W, Bechaux C, Darney K, Grech A, Brochot C, 3 Beaudouin R, Bois FY, Ragas A, Lautz L, Oldenkamp R, Kramer N, Kasteel E, Testai E, Vichi S, Di Consiglio E, Turco L, Buratti F, Baas J, Augustine S, Marques G, Kass GE, Reilly L, Richardson J, Gilsenan M, Dujardin B, Verhagen H, de Seze G, Spyropoulos D, Nougadere A, Cortinas-Abrahantes J, Livaniou A, Manini P, Verloo D, Bassan A, Ceriani L, Pavan M, Tebby C, Benfenati E, Paini A, Liem D, Robinson T

Reconnecting exposure, toxicokinetics and toxicity in food safety : OpenFoodTox and TKplate for human health, animal health and ecological risk assessment.

54. Congress of the European Societies of Toxicology (EUROTOX 2018), Sep 2018, Bruxelles, Belgium. pp.S29, □10.1016/j.toxlet.2018.06.1128□

Benfenati E, Manganaro A, Gini G

VEGA-QSAR: AI inside a platform for predictive toxicology

Proceedings of the workshop "Popularize Artificial Intelligence 2013", December 5th 2013, Turin, Italy
Published on CEUR Workshop Proceedings Vol-1107

Ferrari T, Gini G, Golbamaki Bakhtyari N, Benfenati E

Mining toxicity structural alerts from SMILES: A new way to derive structure activity relationships

in: Proc. 2011 IEEE Symposium on Artificial Life (IEEE Symposium Series on Computational Intelligence - SSCI 2011), April 11-15, 2011, Paris, France, IEEE 2011, ISBN: 978-1-4577-0470-3

Benfenati E, Avouris N, Chaudry Q, Chretien J R, Craciun M, Gini G, Lefebvre B, Lemke F, Neagu D, Piclin N, Pintore M, Roncaglioni A

Five candidate models for regulatory use of QSAR for toxicity of pesticides

in: Proceedings of QSAR 2006, Lyon, France, May 8-12, 2006, 76

Pintore M, Piclin N, Wechman C, Roncaglioni A, Benfenati E, Chretien J R

Comparing descriptors and modelling algorithms in ecotoxicity

in: Proceedings of QSAR 2006, Lyon, France, May 8-12, 2006, 30

Mazzatorta P, Benfenati E, Schuller B, Romberg M, McCourt D, Dubitzky W, Sild S, Karelson M, Papp A, Bagyi I, Darvas F

OpenMolGRID: Molecular science and engineering in a Grid context

in: Arabnia H R, Ni J (Eds.), Parallel and distributed processing techniques and applications, Proc. Int. Conf. PDPTA '04, June 21-24, Las Vegas, Nevada, vol. 2,CSREA Press, Las Vegas, USA (2004), 775-779

Lemke F, Mueller J A, Benfenati E

Modelling and prediction of toxicity of environmental pollutants

in: López J A, Benfenati E, Dubitzky W (Eds.), Knowledge Exploration in Life Science Informatics: Int. Symp. KELSI 2004., Milan, Italy, November 25-26, 2004, LNCS vol. 3303, Springer-Verlag GmbH, Berlin, Germany (2004), 221-234

Benfenati E

Modelling aquatic toxicity with advanced computational techniques: Procedures to standardize data and compare models

in: López J A, Benfenati E, Dubitzky W (Eds.), Knowledge Exploration in Life Science Informatics: Int. Symp. KELSI 2004., Milan, Italy, November 25-26, 2004, LNCS vol. 3303, Springer-Verlag GmbH, Berlin, Germany (2004), 235-248

McCourt D, Lopez J, Benfenati E, Mazzatorta P, Romberg M, Schuller B, Dubitzky W

Towards and intelligent data type for toxicity

in: Arabnia H R, Joshua R, Mun Y (Eds.), Artificial Intelligence, Proc. Int. Conf. on Artificial Intelligence, IC-AI 03, June 23-26, 2003, Las Vegas, Nevada, vol. 1, CSREA Press, Las Vegas, USA (2003), 328-334

Gini G, Benfenati E, Neagu C D

Training through European Research Training Networks. Analysis of IMAGETOX

in: Information technology based higher education and training, Proc. 3rd. Int. Conf., Budapest, Hungary, July 4-6, 2002

Gini G, Giumelli M, Benfenati E, Piclin N, Chretien J R, Pintore M

A comparison of probabilistic, neural, and fuzzy modeling in ecotoxicity

in: Proc. 6th Int. Conf. on Knowledge-Based Intelligent Information Engineering Systems and Allied Technologies, Crema, Italy September 16-18, 2002, KES 2002, IOS Press, Amsterdam, The Netherlands (2002), 542-546

Neagu C D, Benfenati E, Gini G, Mazzatorta P, Roncaglioni A

Neuro-fuzzy knowledge representation for toxicity prediction of organic compounds

in: Artificial Intelligence, Proc. 15th. European Conference, Lyon, France, 21-26 July, IOS Press, Amsterdam (2002), 498-502

Benfenati E, Mazzatorta P, Neagu C D, Gini G

Combining classifiers of pesticides toxicity through a neuro-fuzzy approach

in: Roli F, Kittler J (Eds.), Proc. 3rd Int. Workshop on Multiple Classifier Systems, Cagliari, Italy, June 24-26, 2002, MCS 2002, LNCS vol. 2364, Springer-Verlag GmbH, Berlin, Germany (2002), 293-303

Piclin N, Ros F, Pintore M, Benfenati E, Chrétien JR

A database mining tool to assess pesticide toxicity

In: Preprint of extended abstracts. Vol 42 No1. Pp 251-255. Symposia Papers Presented Before the Division of Environmental Chemistry, American Chemical Society, Orlando, FL, April 7-11, 2002

Chrétien JR, Pintore M, Piclin N, Ros F, Benfenati E,

New perspectives in ecotoxicity database mining

In: Preprint of extended abstracts. Vol 42 No1. Pp 256-260, Symposia Papers Presented Before the Division of Environmental Chemistry, American Chemical Society, Orlando, FL, April 7-11, 2002

Abba L, Gini G, Benfenati E

Results from a data mining approach to predictive toxicology. The case of pesticide data

in: Pattern Recognition in Information Systems, Proc. 2nd. Int. Workshop, Alicante, Spain, April 2-3, 2002

Gini G, Lorenzini M, Benfenati E, Brambilla R, Malvé L

Mixing a symbolic and a subsymbolic expert to improve carcinogenicity prediction of aromatic compounds

in: Roli F, Kittler J (Eds.), Proc. 2nd Int. Workshop on Multiple Classifier Systems, Cambridge, UK, July 2-4, 2001, MCS 2001, LNCS vol. 2096, Springer-Verlag GmbH, Berlin, Germany (2001), 126-135

Renners I, Grauel A, Ludwig L A, Benfenati E, Pelagatti S, Robert D, Carbo-Dorca R, Girones X

Modeling toxicity with molecular descriptors and similarity measures via B-spline networks

in: Information Processing Management Uncertainty in Knowledge-Based Systems, 8th. Int. Conf., Madrid, July 3-7, 2000, vol. II

Gini G, Benfenati E, Boley D

Clustering and classification techniques to assess aquatic toxicity

in: Knowledge-based intelligent engineering system & allied technologies, 4th. Int. Conference, Brighton UK, 30 Aug.-1 Sept., Institute Electrical Electronics Engineers, Piscataway NJ (2000), 166-172

Gini G, Balestri M, Benfenati E, Pelagatti S

Prediction of ecotoxicity of pesticides: Comparison of multivariate analysis, neural networks, and classifiers

in: Artificial Intelligence and Mathematics, Sixt Int: Symp. Fort Lauderdale, FL, Jan. 5-7, 2000.

http://rutcor.rutgers.edu/-amai/top.html

Benfenati E, Pelagatti S, Grasso P, Gini G

COMET: the approach of a project in evaluating toxicity

in: Predictive Toxicology of Chemicals: Experiences and Impact of AI Tools, Papers from 1999 AAAI Spring Symposium, Stanford, March 22-24, 1999, The AAAI Press, Menlo Park CA, USA (1999), 40-43

Darvas F, Papp A, Allerdyce A, Benfenati E, Gini G, Tichy M, Sobb N, Citti A

Overview of different artificial intelligence approaches combined with a deductive logic-based expert system for predicting chemical toxicity

in: Predictive Toxicology of Chemicals: Experiences and Impact of AI Tools, Papers from 1999 AAAI Spring Symposium, Stanford, March 22-24, 1999, The AAAI Press, Menlo Park CA, USA (1999), 94-99

Gini G, Benfenati E

What experiments are suitable to access the prediction of toxic effects of chemicals?

in: Artificial Intelligence, Sixth Int. Joint Conference, Workshop on EMP Empirical AI Achim Hoffman, Stockholm, Sweden, Jul. 31-Aug: 6, 1999

Gini G, Benfenati E, Grasso P, Lorenzini M

Predictive toxicology results integrating different AI paradigms: the carcinogenicity case

in: Intelligent Industrial Automation-IIA'99, Soft Computing-SOCO'99, Proc. third Int. ICSC Symp., Genova, June 1-4, ICSC, Canada/Switzerland (1999)

Fanelli R, Mariani G, Fattore E, Benfenati E

Dioxin concentrations in the atmosphere over Seveso

in: Ballarin-Denti A (Ed.), Chemistry, Man and Environment. The Seveso Accident 20 years on: Monitoring, Epidemiology and Remediation, Proc. Int. Meeting, Milan, Italy, October 21-22, 1996, Elsevier Science Ltd, Amsterdam, The Netherlands (1999), 127-137

Fattore E, Benfenati E, Mariani G, Guzzi A, Mangiapan S, Fanelli R

Air levels of dioxins at Seveso: Patterns and sources

in: Dioxin '99, 19th. Int. Symp. on Halogenated Environmental Organic Pollutants and POPs, Venezia, 12-17 sett. 1999, Emmezeta Congressi, Milano (1999), 315-318

Benfenati E, Pierucci P, Fanelli R, Preiss A, Levsen K

Quantitation of nonylphenols in an industrial textile effluent using GCMS and LC-NMR

in: Dioxin '99, 19th. Int. Symp. on Halogenated Environmental Organic Pollutants and POPs, Venezia, 12-17 sett. 1999, Emmezeta Congressi, Milano (1999), 55-58

Gini G, Lorenzini M, Vittore A, Benfenati E, Grasso P

Some results for the prediction of carcinogenicity using hybrid systems

in: Predictive Toxicology of Chemicals: Experiences and Impact of AI Tools, Papers from 1999 AAAI Spring Symposium, Stanford, March 22-24, 1999, The AAAI Press, Menlo Park CA, USA (1999), 139-143

Fattore E, Mariani G, Guzzi A, Di Guardo A, Benfenati E, Lodi M, Fanelli R

Air dioxin concentrations in Seveso area

in: Halogenated Environmental Organic Pollutants, 18th. Symp., Stockholm, Sweden, August 17-21, 1998

Levsen K, Buscher W, Peters R, Benfenati E

Development of new instrumental metyhods for on-site monitoring of industrial waste water

in: Waste water treatment and monitoring, abatement of emissions to the atmosphere, cleaner technologies, European Workshop environmental technologies; Cranfield University, Cranfield UK (1998), 73-76

Benfenati E, Barceló D, Johnson I, Galassi S, Levsen K

Protocol for the evaluation of residues in industrial contaminated liquid effluents (PERICLES)

in: Waste water treatment and monitoring, abatement of emissions to the atmosphere, cleaner technologies, European Workshop environmental technologies, Cranfield University, Cranfield UK (1998), 79-83

Benfenati E

Protocol for the evaluation of residues in industrial contaminated liquid effluents - PERICLES

in: European Workshop on environmental technologies 1996, Copenhagen (DK), November 13-15, 1996, Carthaus J F, Bonn (1997), 165-174

Benfenati E, Mangiapan S, Grasso P, Galassi S, Provini A, Barceló D, Terreni M, Pregnolato M, Gini G

Biodegradation of pesticides in water: Alachlor, a special case

in: Environmental workshop on on-line monitoring of micropollutants in aquatic systems, Report EUR 16758 EN, European Commission, Bruxelles (1996), 47-53

Benfenati E, Barceló D, Johnson I, Galassi S, Levsen K

Protocol for the evaluation of residues in industrial contaminated liquid effluents - PERICLES

in: Environmental technologies, European workshop 1996, GFA, Hennef, Denmark (1996), 167-174

Benfenati E, Facchini G, Carezzi F, Fanelli R

Mass spectrometry for quality control of groundwater pollution from landfills

in: Reichard E G, Zapponi G A (Eds.), Assessing and Managing Health Risks from Drinking Water

Contamination: Approaches and Applications, Proc. 1st Int. Symp., Rome, Italy, Sept. 13-17, 1994, IAHS Press, 233, Wallingford, UK (1995), 311-313

Benfenati E, Mangiapan S, Terreni M, Vassalli O, Grasso P, Galassi S, Provini A

Mass spectrometric studies of the metabolism of alachlor and metolachlor in water

in: Reichard E G, Zapponi G A (Eds.), Assessing and Managing Health Risks from Drinking Water

Contamination: Approaches and Applications, Proc. 1st Int. Symp., Rome, Italy, Sept. 13-17, 1994, IAHS Press, 233, Wallingford, UK (1995), 324-326

Van Loosdrecht M, Barceló D, Benfenati E, Bianchedi R, Coccagna L, Fernex F, Maslejova A, Ramadori R, Rindone B, Sipos L

Urban and industrial waste water

in: Depollution planning of mediterranean sea. Recommendations for a sound policy, S.Miniato (Pisa), Oct. 22-24, 1992, CNR, Roma (1992), 17-27

Benfenati E, Chen S, Fanelli R, Icardi G

Synthesis of a deuterated analog of Leu-enkephalin for FAB quantitative analysis

in: Proc. 36th ASMS Conference on Mass Spectrometry and Allied Topics, San Francisco, California, June 5-10, 1988, 417-418

Davoli E, Mariani G, Benfenati E, Fanelli R

HRGC-MS measurement of plasma nicotine levels after smoking or chewing nicotine gums

in: Proc. 36th ASMS Conference on Mass Spectrometry and Allied Topics, San Francisco, California, June 5-10, 1988, 1022-1023

Benfenati E, Bettazzoli L, Chen S, De Bellis G, Fanelli R, Pege G

Quantitative analysis of lysophosphatidylserine (LPS) by FAB-MS

in: Proc. 36th ASMS Conference on Mass Spectrometry and Allied Topics, San Francisco, California, June 5-10, 1988, 873-874

Benfenati E, Bettazzoli L, Davoli E, Gavinelli M, Macconi D, Noris M

Mass spectrometric analysis of platelet activating factor (PAF) in mouse urine

in: Proc. 36th ASMS Conference on Mass Spectrometry and Allied Topics, San Francisco, California, June 5-10, 1988, 871-872

Valcavi U, Bosone E, Farina P, Castelli M G, Chiabrando C, Benfenati E

Identification of urinary metabolism of 9-hydroxy-19,20-bis-nor-prostanoic acid (rosaprostol)

in: Todd J F J (Ed.), Advances in mass spectrometry 1985 - Part B: Proc. 10th int. mass spectrometry conf., Swansea, UK, September 9-13, 1985, John Wiley & Sons, Chichester, UK (1986), 707-708

Benfenati E, Cazzola D, Carlucci G, Manna L, Fanelli R, Airoldi L

Electron impact mass spectra of fluoroacyl derivatives of some diarylamines and their quantitative analysis in rubber industry workers' urine

in: Todd J F J (Ed.), Advances in mass spectrometry 1985 - Part B: Proc. 10th int. mass spectrometry conf., Swansea, UK, September 9-13, 1985, John Wiley & Sons, Chichester, UK (1986), 1273-1274

Books edited:

Benfenati E (Ed.)

In silico Methods for Predicting Drug Toxicity. Second Edition.

Springer, New York, USA (2022), pp 1-680.

Benfenati E (Ed.)

In silico Methods for Predicting Drug Toxicity

Springer, New York, USA (2016), pp 1-483.

Benfenati E (Ed.)

Quantitative Structure-Activity Relationships (QSAR) for Pesticide Regulatory Purposes

Elsevier Science Ltd, Amsterdam, The Netherlands (2007)

López J A, Benfenati E, Dubitzky W (Eds.)

Knowledge Exploration in Life Science Informatics: Int. Symp. KELSI 2004., Milan, Italy, November 25-26, 2004

LNCS vol. 3303, Springer-Verlag GmbH, Berlin, Germany (2004)

Projects

EU funded projects

as *coordinator:*

1. Strengthen OpenFoodTox development for the Evaluation and Risk Assessment of substances (**sOFT-ERA**). EFSA funded project: OC/EFSA/iDATA/2022/02, 2022-2026.
2. Concerting experimental data and in silico models for REACH (**LIFE CONCERT REACH)**. LIFE17 GIE/IT/000461. 2018-2022.
3. Further development and update of EFSA's Chemical Hazards (**OptiTox**). OC/EFSA/SCER/2018/01.2018-2022.
4. Integrating VEGA, toxRead, MERLIN-Expo and ERICA in a platform for risk assessment and substitution for risky substances (**LIFE**-**VERMEER**), LIFE16ENV/IT7000167, 2017-2022.
5. Promoting the use of in silico methods in industry (**LIFE PROSIL**), LIFE12 ENV/IT/000154, 2013-2016.
6. Research assistance on the development of *in silico* tools for human and ecological risk assessment of chemicals. EFSA Contract NP/EFSA/AFSCO/2016/01, 2016.
7. Chemical Assessment according to Legislation Enhancing the In silico DOcumentation and Safe use (**CALEIDOS**), LIFE11 ENV/IT/000295, 2013-2015.
8. ToxBank: Supporting Integrated Data Analysis and Servicing of Alternative Testing Methods in Toxicology (**TOXBANK**), 267042, 2011-2015.
9. Alternative Non-Testing methods Assessed for REACH Substances (**ANTARES**), LIFE08 ENV/IT/000435, 2010-2012
10. Organising dissemination on Results of projects on Chemical Evaluation, Spreading Techniques for Risk Assessment (**ORCHESTRA**), 226521, 2009-2012
11. Development of Freely Available Predictive Models Based on Simple Chemical Descriptors (**CHEMPREDICT**), MIF1-CT-2006-039036, 2007-2010
12. Computer Assisted Evaluation of industrial chemical Substances According to Regulations (**CAESAR**), 022674 (SSPI), 2006-2009
13. Structure-activity relationships leading experts in mutagencity and carcinogenicity (**SCARLET**), SP5A-CT-2007-044166, 2007-2008
14. Research on Animal and In-vitro studies and Numerical methods: Bridging Opportunities through a Workshop (**RAINBOW**), LSSB-CT-2005-018695, 2006-2007
15. Development of Environmental Modules for Evaluation of Toxicity of pesticide Residues in Agriculture (**DEMETRA**), QLK5-CT-2002-00691, 2003-2006
16. Validation of selected, non-commercial (Q)SAR models for estrogen receptor and androgen receptor binding. European Commission, JRC. CCR.IHCP.C43041.X0. 2005.
17. Intelligent Modeling Algorithms for the General Evaluation of Toxicity (**IMAGETOX**), HPRN-CT-1999-00015, 2000-2004
18. COmputerized Molecular Evaluation of Toxicity (**COMET**), PL970802, 1998-2001
19. Development and validation of immunoanalytical methods for the determination of plant protection products and related compounds (ERBIC15CT960802)
20. Protocol for the Evaluation of Residues in Industrial Contaminated Liquid EffluentS (**PERICLES**), ENV4-CT95-0021, 1996-1999
21. Development of multiresidue HPLC method for the determination of environmentally important pesticides in water, CIPD 925097, 1993-1996
22. Analysis of pesticides and their degradation products - An integrated study, EV5V-CT92-0061, 1992-1995

as *participant:*

1. **PollinERA –** Understanding pesticide-Pollinator interactions to support EU Environmental Risk Assessment and policy (Horizon project 101135005 - GAP-101135005)**.** 2024-2027
2. **PARC** – Partnership for the Assessment of Risks from Chemicals. Horizon project. 2022-2029. Grant agreement 101057014.
3. Nanoparticle emissions from the transport sectors (**nPETS**). H2020. 2021-2024. Grant agreement ID: 954377. 2021-2024.
4. Ontology-driven and artificial intelligence- of based repeated dose toxicity testing chemicals for next generation risk assessment (**ONTOX**). H2020-963845. 2021-2025.
5. Prioritisation and Risk Evaluation of Medicines in the EnviRonment (**PREMIER**). IMI2 JU. 2020-2026.
6. Advance machine learning for Innovative Drug Discovery (**AIDD**). H2020. 2020-2024.
7. An iterative strategy of testing systems for identification of EDs related to metabolic disorders (**OBERON**). H2020, SC1-BHC. 825712. 2019-2023.
8. **In3**. An integrated interdisciplinary approach to animal-free chemical and nanomaterial safety assessment. H2020- 721975. 2017-2021.
9. COMputational tool for the assessment and substitution of Biocidal Active substanceS of Ecotoxicological concern **(LIFE-COMBASE**), LIFE15 ENV/ES/000416.
10. An integrated European "flagship" program driving mechanism-based toxicity testing and risk assessment for the 21st century (**EU-ToxRisk**). H2020- 681002. 2016-2021.
11. Design of polyPEPTIdes diblock copolymers as emulsifiers to produce safe, controlled and reliable novel stimuli-responsive nanoCAPSules for skin care applications (**PEPTICAPS**), H2020-NMP-PILOTS-2015, 686141, 2015-2018.
12. a LOW environmental impact BRAke SYStem (**LOWBRASYS**), H2020-MG-2014-2015, 636592, 2015-2018.
13. InREACH: protecting health and environment by streamlining REACH compliance check at European Economic Area import stage (**InREACH**), LIFE13 ENV/IT/000849, 2014-2017
14. Cementitious brake control (**COBRA**), LIFE13 ENV/IT/000492, 2014-2018

15. Endocrine Disruptors in silico/in vitro Evaluation and Substitution for Industrial Applications (**EDESIA**), LIFE2012 000633, 2013-2015
16. Predicting toxicology of engineered nanoparticles (**PreNanoTox**), 309666, 2013-2015
17. Modelling properties, interactions, toxicity and environmental behaviour of engineered nanoparticles (**NanoPUZZLES**), 309837, 2013-2015
18. Building bridges between specialists in computational and empirical risk assessment of engineered nanomaterials (**NanoBRIDGES**), PIRSES-GA-2011-295128, 2012-2014
19. Risk-based management of chemicals and products in a circular economy at a global scale (**RISKCYCLE**), 226552, 2010-2012
20. Optimized Strategies for Risk Assessment of Industrial Chemicals based on Intelligent Combinations of Non-Test and Test Information (**OSIRIS**), 037017 (GOCE), 2007-2011
21. Grid services based environment to enable innovative research (**CHEMOMENTUM**), FP6-2005-IST-5-033437, 2006-2008
22. Chemical Food Safety Network for the enlarging Europe (**SAFEFOODNET**), FOOD-CT-2004-513988, 2005-2007
23. Chemicals as contaminants in the food chain: a network of excellence for research, risk assessment and education (**CASCADE**), FOOD-CT-2004-506319, 2004-2009
24. Harmonised environmental indicators for pesticide risk (**HAIR**), SSPE-CT-2003-501997, 2004-2007
25. Concerted Action to develop a European Framework for probabilistic risk assessment of the environmental impacts of pesticides (**EUFRAM**), QLK5- CT-2002-01346, 2003-2006
26. Environmental Agent Susceptibility Assessment utilising existing and novel biomarkers as Rapid non-Invasive testing methods (**EASYRING**), QLK4-CT-2002-02286, 2003-2005
27. Open Computing GRID for Molecular Science and Engineering (**OpenMolGRID**), IST-2001-37238, 2002-2005
28. Knowledge and exploitation in science and technology (**COST 282**), 2001-2005
29. Fate and toxicity of allelochemicals (natural plant toxins) in relation to environment and consumer (**FATEALLCHEM**), QLRT-2000-01967, 2001-2004
30. Multichannel electrochemical biosensor for rapid food safety monitoring (**MEBFOOD**), IC15-CT98-0910, 1998-2001
31. Development of new instrumental methods for on-site monitoring of industrial wastewater, ENV4-CT95-0020, 1996-1999
32. Certification of PCDD/PCDF in soils, MAT1 CT930045, 1995-1996
33. Development of second-generation expert systems for environmental toxicology, CP 1029, 1995-1998.
34. Polychlorinated dibenzo(p)dioxins and dibenzofurans in municipal waste incinerator fly ash, Certification of CRM 490, BCR project, 1986-1994

Other international projects, as coordinator

- toDIVINE, "to optimize Databases and Innovative Virtual models: Integrating Non-testing methods for Environmental properties". Project funded by the German UBA, 2017-2019.
- JANUS, "Joining environmental, ecotoxicological and toxicological Assessment of chemical substances with Non-testing methods within a Unified Screening". Project funded by the German UBA, 2016-2018.
- PROMETHEUS, PRioritization Of chemicals: a METHodology Embracing PBT parameters into a Unified Strategy. Project funded by the German UBA, 2013-2015.
- Validation of Selected, Non - Commercial (Q)SAR Models for Estrogen Receptor and Androgen Receptor Binding. Project funded by the JRC. 2005.
- NATO project on "Molecular descriptors and advanced computing in carcinogenicity prediction", 1998-2000
- "Mass spectrometry in the analysis of phospholipids ", a bilateral two-year project funded by CNR (Consiglio Nazionale delle Ricerche), Rome, Italy, and University of Colorado Denver, Denver CO, U.S.A., 1989-1990
- "Study on cardiac metabolism by mass spectrometry and NMR", a bilateral three-year project funded by CNR (Consiglio Nazionale delle Ricerche), Rome, Italy, and Stanford University School of Medicine, Stanford CA, U.S.A., 1985-1987

National projects, as coordinator

- Evaluation of alternatives to PFAS. Bibliographic search, and in silico modelling of candidate substitutes of PFAS. Project funded by the Ministero dell'Ambiente, della Tutela del Territorio e del Mare (MATTM), Rome, Italy, 2018.
- Development of a general method to identify candidate substances for substitution of CMR. Project funded by Istituto Superiore di Sanità, Rome, Italy, 2018.
- Working group on QSAR models for REACH. Project funded by Istituto Superiore di Sanità, Rome, Italy, 2012-2013.

Memberships

2010 - 2022 Member of the External Science Advisory Panel of CEFIC, the European Chemical Industry Council, Brussels, Belgium.

2015 - 2017 Member of the Working Group on Weight of Evidence of the European Food Safety Authority, Parma, Italy

2017 – current, Member of the Advisory Group on Molecular Screening and Toxicogenomics (EAGMST) of the OECD, Paris, France.

2017 - 2019 Member of the Working Group on Chemical Mixtures of the European Food Safety Authority, Parma, Italy

2019 – current, Member of the Cross Cutting Working Group on Chemical Mixtures of the European Food Safety Authority, Parma, Italy

2019 – 2020, Member of the Working Group on Food Contact Materials of the European Food Safety Authority, Parma, Italy

2021-current. Member of the Working Group on Botanicals of the European Food Safety Authority, Parma, Italy

2022-current. External expert of the Scientific Committee on the Consumers Safety of the European Commission.

2022-current. Member of the Working Group on Read-across of the European Food Safety Authority, Parma, Italy

2022-current. Member of the Working Group on NAMS for pesticide metabolites of the European Food Safety Authority, Parma, Italy

E. Benfenati is in the editorial board of the scientific journals:

- • ALTEX
- • BMC Chemistry
- • Toxics

- • Journal of Environmental Science and Health, Part C
- • Cosmetic Technology
- • Review Editor in *Frontiers in Pharmacology* - section Experimental Pharmacology and Drug Discovery
- • Review Editor in *Frontiers in Pharmacology* - section Predictive Toxicology

Other Relevant Information