Emilio Benfenati

List of Publications by Year in Descending Order

493 papers	10,928 citations	47 h-index	77 g-index
536 ext. papers	12,303 ext. citations	5.1 avg, IF	6.41 L-index

#	Paper	IF	Citations
493	Skin sensitization quantitative QSAR models based on mechanistic structural alerts.. *Toxicology*, **2022**, 153111	4.4	
492	The system of self-consistent models for vapour pressure. *Chemical Physics Letters*, **2022**, 790, 139354	2.5	2
491	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*, **2022**, 423, 127236	12.8	6
490	Patent Toxicity. *Research Policy*, **2022**, 51, 104329	7.5	1
489	In Silico Methods for Carcinogenicity Assessment.. *Methods in Molecular Biology*, **2022**, 2425, 201-215	1.4	0
488	Using VEGAHUB Within a Weight-of-Evidence Strategy.. *Methods in Molecular Biology*, **2022**, 2425, 479-495	1.4	
487	In Silico Models for Repeated-Dose Toxicity (RDT): Prediction of the No Observed Adverse Effect Level (NOAEL) and Lowest Observed Adverse Effect Level (LOAEL) for Drugs.. *Methods in Molecular Biology*, **2022**, 2425, 241-258	1.4	0
486	In Silico Prediction of Chemically Induced Mutagenicity: A Weight of Evidence Approach Integrating Information from QSAR Models and Read-Across Predictions.. *Methods in Molecular Biology*, **2022**, 2425, 149-183	1.4	0
485	In Silico Models for Developmental Toxicity.. *Methods in Molecular Biology*, **2022**, 2425, 217-240	1.4	
484	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*, **2022**, 23,	6.3	1
483	The VEGAHUB Platform: The Philosophy and the Tools.. *ATLA Alternatives To Laboratory Animals*, **2022**, 2611929221090530	2.1	0
482	Exploration of structural requirements for azole chemicals towards human aromatase CYP19A1 activity: Classification modeling, structure-activity relationships and read-across study.. *Toxicology in Vitro*, **2022**, 105332	3.6	2
481	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*, **2022**, 830, 154795	10.2	0
480	Development of new QSAR models for water, sediment, and soil half-life. *Science of the Total Environment*, **2022**, 156004	10.2	1
479	Modeling the migration of chemicals from food contact materials to food: The MERLIN-expo/SPHERA toolbox. *Food and Chemical Toxicology*, **2022**, 113118	4.7	
478	From Data to Models **2021**, 89-124		
477	Computational Tools for the Assessment and Substitution of Biocidal Active Substances of Ecotoxicological Concern **2021**, 527-546		

476	Green Chemistry in the Synthesis of Pharmaceuticals.. *Chemical Reviews*, **2021**,	68.1	22
475	The Tools for Aquatic Toxicology within the VEGAHUB System **2021**, 493-511		
474	The system of self-consistent semi-correlations as one of the tools of cheminformatics for designing antiviral drugs. *New Journal of Chemistry*, **2021**, 45, 20713-20720	3.6	2
473	Maintenance, update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0. *EFSA Supporting Publications*, **2021**, 18, 6476E	1.1	1
472	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**, 26,	4.8	1
471	The Monte Carlo method to build up models of the hydrolysis half-lives of organic compounds. *SAR and QSAR in Environmental Research*, **2021**, 32, 463-471	3.5	5
470	CATMoS: Collaborative Acute Toxicity Modeling Suite. *Environmental Health Perspectives*, **2021**, 129, 47013	8.4	14
469	The self-organizing vector of atom-pairs proportions: use to develop models for melting points. *Structural Chemistry*, **2021**, 32, 967-971	1.8	3
468	A descriptor-based analysis to highlight the mechanistic rationale of mutagenicity. *Journal of Environmental Science and Health, Part C: Toxicology and Carcinogenesis*, **2021**, 1-24	1.6	
467	Safer chemicals using less animals: kick-off of the European ONTOX project. *Toxicology*, **2021**, 458, 152846	4.4	10
466	The index of ideality of correlation improves the predictive potential of models of the antioxidant activity of tripeptides from frog skin (Litoria rubella). *Computers in Biology and Medicine*, **2021**, 133, 104370	7	6
465	The QSAR-search of effective agents towards coronaviruses applying the Monte Carlo method. *SAR and QSAR in Environmental Research*, **2021**, 32, 689-698	3.5	1
464	Pesticides, cosmetics, drugs: identical and opposite influences of various molecular features as measures of endpoints similarity and dissimilarity. *Molecular Diversity*, **2021**, 25, 1137-1144	3.1	2
463	Integrated 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, 247-257	4	5
462	Towards a systematic use of effect biomarkers in population and occupational biomonitoring. *Environment International*, **2021**, 146, 106257	12.9	17
461	EFSA's OpenFoodTox: An open source toxicological database on chemicals in food and feed and its future developments. *Environment International*, **2021**, 146, 106293	12.9	19
460	First report on chemometric modeling of hydrolysis half-lives of organic chemicals. *Environmental Science and Pollution Research*, **2021**, 28, 1627-1642	5.1	4
459	SpheraCosmolife: a new tool for the risk assessment of cosmetic products. *ALTEX: Alternatives To Animal Experimentation*, **2021**, 38, 565-579	4.3	2

458	Paradox of 'ideal correlations': improved model for air half-life of persistent organic pollutants. *Environmental Technology (United Kingdom)*, **2021**, 1-6	2.6	3
457	Quantitative Structure-Activity Relationship Modeling of the Amplex Ultrared Assay to Predict Thyroperoxidase Inhibitory Activity. *Frontiers in Pharmacology*, **2021**, 12, 713037	5.6	2
456	Ecotoxicological QSAR modeling of the acute toxicity of organic compounds to the freshwater crustacean Thamnocephalus platyurus. *Chemosphere*, **2021**, 280, 130652	8.4	4
455	Semi-correlations as a tool to model for skin sensitization. *Food and Chemical Toxicology*, **2021**, 157, 112580	4.7	0
454	Guidance Document on Scientific criteria for grouping chemicals into assessment groups for human risk assessment of combined exposure to multiple chemicals.. *EFSA Journal*, **2021**, 19, e07033	2.3	6
453	Structures of Endocrine-Disrupting Chemicals Correlate with the Activation of 12 Classic Nuclear Receptors. *Environmental Science & Technology*, **2021**,	10.3	5
452	Maintenance,update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0. *EFSA Supporting Publications*, **2020**, 17, 1822E	1.1	3
451	New QSAR models to predict chromosome damaging potential based on the in vivo micronucleus test. *Toxicology Letters*, **2020**, 329, 80-84	4.4	4
450	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*, **2020**, 735, 139243	10.2	12
449	Homology Modeling of the Human P-glycoprotein (ABCB1) and Insights into Ligand Binding through Molecular Docking Studies. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	12
448	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	2.3	3
447	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	5.1	16
446	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. *Environmental Health Perspectives*, **2020**, 128, 27002	8.4	70
445	Ecotoxicological effects of atmospheric particulate produced by braking systems on aquatic and edaphic organisms. *Environment International*, **2020**, 137, 105564	12.9	6
444	Value and limitation of structure-based profilers to characterize developmental and reproductive toxicity potential. *Archives of Toxicology*, **2020**, 94, 939-954	5.8	0
443	Towards an Understanding of the Mode of Action of Human Aromatase Activity for Azoles through Quantum Chemical Descriptors-Based Regression and Structure Activity Relationship Modeling Analysis. *Molecules*, **2020**, 25,	4.8	8
442	QSAR models for biocides: The example of the prediction of acute toxicity. *SAR and QSAR in Environmental Research*, **2020**, 31, 227-243	3.5	18
441	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	1.8	2

440	Internationalization of read-across as a validated new approach method (NAM) for regulatory toxicology. *ALTEX: Alternatives To Animal Experimentation*, **2020**, 37, 579-606	4.3	27
439	Automated integration of structural, biological and metabolic similarities to improve read-across. *ALTEX: Alternatives To Animal Experimentation*, **2020**, 37, 469-481	4.3	6
438	QSAR Models for Human Carcinogenicity: An Assessment Based on Oral and Inhalation Slope Factors. *Molecules*, **2020**, 26,	4.8	6
437	QSAR-Models, Validation, and IIC-Paradox for Drug Toxicity. *International Journal of Quantitative Structure-Property Relationships*, **2020**, 5, 22-43	1.2	1
436	Ecotoxicological assessment of pharmaceuticals and personal care products using predictive toxicology approaches. *Green Chemistry*, **2020**, 22, 1458-1516	10	36
435	Exploring QSAR modeling of toxicity of chemicals on earthworm. *Ecotoxicology and Environmental Safety*, **2020**, 190, 110067	7	16
434	Use of the index of ideality of correlation to improve aquatic solubility model. *Journal of Molecular Graphics and Modelling*, **2020**, 96, 107525	2.8	11
433	First report on a classification-based QSAR model for chemical toxicity to earthworm. *Journal of Hazardous Materials*, **2020**, 386, 121660	12.8	14
432	New in silico models to predict in vitro micronucleus induction as marker of genotoxicity. *Journal of Hazardous Materials*, **2020**, 385, 121638	12.8	8
431	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	10.2	21
430	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	3.5	2
429	Zebrafish AC modelling: (Q)SAR models to predict developmental toxicity in zebrafish embryo. *Ecotoxicology and Environmental Safety*, **2020**, 202, 110936	7	5
428	QSAR model for pesticides toxicity to Rainbow Trout based on "ideal correlations". *Aquatic Toxicology*, **2020**, 227, 105589	5.1	8
427	Ecosystem ecology: Models for acute toxicity of pesticides towards Daphnia magna. *Environmental Toxicology and Pharmacology*, **2020**, 80, 103459	5.8	6
426	Structures of Endocrine-Disrupting Chemicals Determine Binding to and Activation of the Estrogen Receptor and Androgen Receptor. *Environmental Science & Technology*, **2020**, 54, 11424-11433	10.3	16
425	'Ideal correlations' for the predictive toxicity to. *Toxicology Mechanisms and Methods*, **2020**, 30, 605-610	3.6	5
424	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*, **2020**, 205, 111291	7	3
423	Modelling quantitative structure activity-activity relationships (QSAARs): auto-pass-pass, a new approach to fill data gaps in environmental risk assessment under the REACH regulation. *SAR and QSAR in Environmental Research*, **2020**, 31, 785-801	3.5	3

422	Prediction of No Observed Adverse Effect Concentration for inhalation toxicity using Monte Carlo approach. *SAR and QSAR in Environmental Research*, **2020**, 31, 1-12	3.5	6
421	Chemometric modeling to predict air half-life of persistent organic pollutants (POPs). *Journal of Hazardous Materials*, **2020**, 382, 121035	12.8	9
420	The index of ideality of correlation: models for flammability of binary liquid mixtures. *Chemical Papers*, **2020**, 74, 601-609	1.9	13
419	VEGAHUB for Ecotoxicological QSAR Modeling. *Methods in Pharmacology and Toxicology*, **2020**, 759-787	1.1	5
418	SAR and QSAR modeling of a large collection of LD rat acute oral toxicity data. *Journal of Cheminformatics*, **2019**, 11, 58	8.6	34
417	Integrating in silico models for the prediction of mutagenicity (Ames test) of botanical ingredients of cosmetics. *Computational Toxicology*, **2019**, 12, 100108	3.1	3
416	Could deep learning in neural networks improve the QSAR models?. *SAR and QSAR in Environmental Research*, **2019**, 30, 617-642	3.5	17
415	Integrating in silico models and read-across methods for predicting toxicity of chemicals: A step-wise strategy. *Environment International*, **2019**, 131, 105060	12.9	43
414	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	3.5	16
413	Integrating QSAR, Read-Across, and Screening Tools: The VEGAHUB Platform as an Example. *Challenges and Advances in Computational Chemistry and Physics*, **2019**, 365-381	0.7	3
412	Guidance on harmonised methodologies for human health, animal health and ecological risk assessment of combined exposure to multiple chemicals. *EFSA Journal*, **2019**, 17, e05634	2.3	100
411	Ecotoxicological QSAR modeling of organic compounds against fish: Application of fragment based descriptors in feature analysis. *Aquatic Toxicology*, **2019**, 212, 162-174	5.1	22
410	QSAR modeling of Daphnia magna and fish toxicities of biocides using 2D descriptors. *Chemosphere* , **2019**, 229, 8-17	8.4	47
409	Methodology of aiQSAR: a group-specific approach to QSAR modelling. *Journal of Cheminformatics*, **2019**, 11, 27	8.6	9
408	The Index of Ideality of Correlation: QSAR Model of Acute Toxicity for Zebrafish (Danio rerio) Embryo. *International Journal of Environmental Research*, **2019**, 13, 387-394	2.9	7
407	Ecotoxicological QSAR modeling of endocrine disruptor chemicals. *Journal of Hazardous Materials*, **2019**, 369, 707-718	12.8	33
406	Chemometric modeling of Daphnia magna toxicity of agrochemicals. *Chemosphere*, **2019**, 224, 470-479	8.4	28
405	CORAL: Building up QSAR models for the chromosome aberration test. *Saudi Journal of Biological Sciences*, **2019**, 26, 1101-1106	4	15

404	QSPR as a random event: solubility of fullerenes C[60] and C[70]. *Fullerenes Nanotubes and Carbon Nanostructures*, **2019**, 27, 816-821	1.8	5
403	Ensemble-Based Modeling of Chemical Compounds with Antimalarial Activity. *Current Topics in Medicinal Chemistry*, **2019**, 19, 957-969	3	6
402	In silico model for mutagenicity (Ames test), taking into account metabolism. *Mutagenesis*, **2019**, 34, 41-48	2.8	6
401	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	12.9	33
400	Virtual Screening of Anti-Cancer Compounds: Application of Monte Carlo Technique. *Anti-Cancer Agents in Medicinal Chemistry*, **2019**, 19, 148-153	2.2	3
399	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	0.4	1
398	Development, validation and integration of in silico models to identify androgen active chemicals. *Chemosphere*, **2019**, 220, 204-215	8.4	17
397	Impact of REACH legislation on the production and importation of CMR (carcinogen, mutagen and reproductive) and explosive chemicals in Italy from 2011 to 2015. *Regulatory Toxicology and Pharmacology*, **2019**, 101, 166-171	3.4	1
396	Investigating landfill leachate toxicity in vitro: A review of cell models and endpoints. *Environment International*, **2019**, 122, 21-30	12.9	46
395	Semi-correlations as a tool to build up categorical (active/inactive) model of GABAA receptor modulator activity. *Structural Chemistry*, **2019**, 30, 853-861	1.8	6
394	Phytotoxicity of wear debris from traditional and innovative brake pads. *Environment International*, **2019**, 123, 156-163	12.9	16
393	Consensus QSAR modeling of toxicity of pharmaceuticals to different aquatic organisms: Ranking and prioritization of the DrugBank database compounds. *Ecotoxicology and Environmental Safety*, **2019**, 168, 287-297	7	57
392	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	2.8	53
391	QSAR Development for Plasma Protein Binding: Influence of the Ionization State. *Pharmaceutical Research*, **2018**, 36, 28	4.5	8
390	Computational Toxicology and Reach **2018**, 245-268		2
389	Mutagenicity, anticancer activity and blood brain barrier: similarity and dissimilarity of molecular alerts. *Toxicology Mechanisms and Methods*, **2018**, 28, 321-327	3.6	8
388	QSPR analysis of threshold of odor for the large number of heterogenic chemicals. *Molecular Diversity*, **2018**, 22, 397-403	3.1	3
387	Use of quasi-SMILES to model biological activity of micelle polymer samples. *Structural Chemistry*, **2018**, 29, 1213-1223	1.8	7

386	Performance of In Silico Models for Mutagenicity Prediction of Food Contact Materials. *Toxicological Sciences*, **2018**, 163, 632-638	4.4	11
385	The application of new HARD-descriptor available from the CORAL software to building up NOAEL models. *Food and Chemical Toxicology*, **2018**, 112, 544-550	4.7	26
384	Perspectives from the NanoSafety Modelling Cluster on the validation criteria for (Q)SAR models used in nanotechnology. *Food and Chemical Toxicology*, **2018**, 112, 478-494	4.7	21
383	A large comparison of integrated SAR/QSAR models of the Ames test for mutagenicity. *SAR and QSAR in Environmental Research*, **2018**, 29, 591-611	3.5	12
382	Quasi-SMILES as a tool to predict removal rates of pharmaceuticals and dyes in sewage. *Chemical Engineering Research and Design*, **2018**, 118, 227-233	5.5	9
381	(Eco)toxicological maps: A new risk assessment method integrating traditional and in silico tools and its application in the Ledra River (Italy). *Environment International*, **2018**, 119, 275-286	12.9	8
380	Classification of a Naïve Bayesian Fingerprint model to predict reproductive toxicity. *SAR and QSAR in Environmental Research*, **2018**, 29, 631-645	3.5	4
379	Genotoxicity induced by metal oxide nanoparticles: a weight of evidence study and effect of particle surface and electronic properties. *Nanotoxicology*, **2018**, 12, 1113-1129	5.3	17
378	Integrated strategy for mutagenicity prediction applied to food contact chemicals. *ALTEX: Alternatives To Animal Experimentation*, **2018**, 35, 169-178	4.3	7
377	A new semi-automated workflow for chemical data retrieval and quality checking for modeling applications. *Journal of Cheminformatics*, **2018**, 10, 60	8.6	34
376	Prediction of antimicrobial activity of large pool of peptides using quasi-SMILES. *BioSystems*, **2018**, 169-170, 5-12	1.9	6
375	SAR for gastro-intestinal absorption and blood-brain barrier permeation of pesticides. *Chemico-Biological Interactions*, **2018**, 290, 1-5	5	7
374	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	10.2	3
373	CORAL: Predictive models for cytotoxicity of functionalized nanozeolites based on quasi-SMILES. *Chemosphere*, **2018**, 210, 52-56	8.4	9
372	Criteria and Application on the Use of Nontesting Methods within a Weight of Evidence Strategy. *Methods in Molecular Biology*, **2018**, 1800, 199-218	1.4	
371	QSAR Modeling of ToxCast Assays Relevant to the Molecular Initiating Events of AOPs Leading to Hepatic Steatosis. *Journal of Chemical Information and Modeling*, **2018**, 58, 1501-1517	6.1	38
370	Prediction of Biochemical Endpoints by the CORAL Software: Prejudices, Paradoxes, and Results. *Methods in Molecular Biology*, **2018**, 1800, 573-583	1.4	3
369	Air quality in the Olona Valley and in vitro human health effects. *Science of the Total Environment*, **2017**, 579, 1929-1939	10.2	11

368	Exposure to PFOA and PFOS and fetal growth: a critical merging of toxicological and epidemiological data. *Critical Reviews in Toxicology*, **2017**, 47, 482-508	5.7	69
367	(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	4.7	14
366	Compilation of Data and Modelling of Nanoparticle Interactions and Toxicity in the NanoPUZZLES Project. *Advances in Experimental Medicine and Biology*, **2017**, 947, 303-324	3.6	4
365	Nano-QSAR Model for Predicting Cell Viability of Human Embryonic Kidney Cells. *Methods in Molecular Biology*, **2017**, 1601, 275-290	1.4	9
364	VOC exposures in California early childhood education environments. *Indoor Air*, **2017**, 27, 609-621	5.4	25
363	Aquatic toxicity of several textile dye formulations: Acute and chronic assays with Daphnia magna and Raphidocelis subcapitata. *Ecotoxicology and Environmental Safety*, **2017**, 144, 79-87	7	52
362	QSAR models for predicting acute toxicity of pesticides in rainbow trout using the CORAL software and EFSA's OpenFoodTox database. *Environmental Toxicology and Pharmacology*, **2017**, 53, 158-163	5.8	42
361	Fragment Prioritization on a Large Mutagenicity Dataset. *Molecular Informatics*, **2017**, 36, 1600133	3.8	9
360	Integrating computational methods to predict mutagenicity of aromatic azo compounds. *Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews*, **2017**, 35, 239-257	4.5	6
359	Guidance on the use of the weight of evidence approach in scientific assessments. *EFSA Journal*, **2017**, 15, e04971	2.3	128
358	Developing innovative in silico models with EFSA's OpenFoodTox database. *EFSA Supporting Publications*, **2017**, 14, 1206E	1.1	8
357	Predicting acute contact toxicity of pesticides in honeybees (Apis mellifera) through a k-nearest neighbor model. *Chemosphere*, **2017**, 166, 438-444	8.4	36
356	Development of Monte Carlo Approaches in Support of Environmental Research. *Challenges and Advances in Computational Chemistry and Physics*, **2017**, 453-469	0.7	2
355	QSPR/QSAR Analyses by Means of the CORAL Software **2017**, 929-955		
354	Nano-QSAR: Model of mutagenicity of fullerene as a mathematical function of different conditions. *Ecotoxicology and Environmental Safety*, **2016**, 124, 32-36	7	33
353	Odor threshold prediction by means of the Monte Carlo method. *Ecotoxicology and Environmental Safety*, **2016**, 133, 390-4	7	8
352	Integrated in silico strategy for PBT assessment and prioritization under REACH. *Environmental Research*, **2016**, 151, 478-492	7.9	22
351	New Quantitative Structure-Activity Relationship Models Improve Predictability of Ames Mutagenicity for Aromatic Azo Compounds. *Toxicological Sciences*, **2016**, 153, 316-26	4.4	19

350	In Silico Methods for Carcinogenicity Assessment. *Methods in Molecular Biology*, **2016**, 1425, 107-19	1.4	9
349	A knowledge-based expert rule system for predicting mutagenicity (Ames test) of aromatic amines and azo compounds. *Toxicology*, **2016**, 370, 20-30	4.4	23
348	Use of Read-Across Tools. *Methods in Molecular Biology*, **2016**, 1425, 305-22	1.4	4
347	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	3.5	6
346	Quantitative structure□ctivity relationship models for bee toxicity. *Toxicological and Environmental Chemistry*, **2016**, 1-12	1.4	2
345	Novel chemical hazard characterisation approaches. *EFSA Journal*, **2016**, 14, e00506	2.3	2
344	In Silico Prediction of Chemically Induced Mutagenicity: How to Use QSAR Models and Interpret Their Results. *Methods in Molecular Biology*, **2016**, 1425, 87-105	1.4	7
343	In Silico Model for Developmental Toxicity: How to Use QSAR Models and Interpret Their Results. *Methods in Molecular Biology*, **2016**, 1425, 139-61	1.4	5
342	A new integrated in silico strategy for the assessment and prioritization of persistence of chemicals under REACH. *Environment International*, **2016**, 88, 250-260	12.9	15
341	Predicting persistence in the sediment compartment with a new automatic software based on the k-Nearest Neighbor (k-NN) algorithm. *Chemosphere*, **2016**, 144, 1624-30	8.4	25
340	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, 453-61	2.8	6
339	New clues on carcinogenicity-related substructures derived from mining two large datasets of chemical compounds. *Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews*, **2016**, 34, 97-113	4.5	16
338	QSAR model for predicting cell viability of human embryonic kidney cells exposed to SiO□ nanoparticles. *Chemosphere*, **2016**, 144, 995-1001	8.4	30
337	QSAR Methods to Screen Endocrine Disruptors. *Nuclear Receptor Research*, **2016**, 3,	1.4	5
336	Toxicology is IN: in silico, in vitro, integrated testing strategy. *ALTEX: Alternatives To Animal Experimentation*, **2016**, 33, 187-8	4.3	1
335	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. *Environmental Health Perspectives*, **2016**, 124, 1023-33	8.4	206
334	QSAR as a Random Event: Selecting of the Molecular Structure for Potential Anti-tuberculosis Agents. *Anti-Infective Agents*, **2016**, 14, 3-10	0.6	6
333	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, 442	5.6	22

332	In Silico Models for Repeated-Dose Toxicity (RDT): Prediction of the No Observed Adverse Effect Level (NOAEL) and Lowest Observed Adverse Effect Level (LOAEL) for Drugs. *Methods in Molecular Biology*, **2016**, 1425, 163-76	1.4	19
331	QSAR Model for Cytotoxicity of Silica Nanoparticles on Human Embryonic Kidney Cells1. *Materials Today: Proceedings*, **2016**, 3, 847-854	1.4	9
330	Quasi-SMILES as a tool to utilize eclectic data for predicting the behavior of nanomaterials. *NanoImpact*, **2016**, 1, 60-64	5.6	18
329	Results of a round-robin exercise on read-across. *SAR and QSAR in Environmental Research*, **2016**, 27, 371-84	3.5	17
328	Classification nano-SAR modeling of metal oxides nanoparticles genotoxicity based on comet assay data. *Toxicology Letters*, **2016**, 258, S271	4.4	3
327	Integrating in silico models to enhance predictivity for developmental toxicity. *Toxicology*, **2016**, 370, 127-137	4.4	23
326	Physiologically based pharmacokinetic modeling of perfluoroalkyl substances in the human body. *Toxicological and Environmental Chemistry*, **2015**, 97, 814-827	1.4	12
325	Chemical characterization and ecotoxicity of three soil foaming agents used in mechanized tunneling. *Journal of Hazardous Materials*, **2015**, 296, 210-220	12.8	23
324	CORAL: Model for octanol/water partition coefficient. *Fluid Phase Equilibria*, **2015**, 397, 44-49	2.5	10
323	Acute phytotoxicity of seven metals alone and in mixture: Are Italian soil threshold concentrations suitable for plant protection?. *Environmental Research*, **2015**, 140, 102-11	7.9	37
322	CORAL: model for no observed adverse effect level (NOAEL). *Molecular Diversity*, **2015**, 19, 563-75	3.1	15
321	Hierarchical Rules for Read-Across and In Silico Models of Mutagenicity. *Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews*, **2015**, 33, 385-403	4.5	7
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