Emilio Benfenati

List of Publications by Citations

Source: https://exaly.com/author-pdf/4299686/emilio-benfenati-publications-by-citations.pdf
Version: 2024-04-28

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	CAESAR models for developmental toxicity. *Chemistry Central Journal*, **2010**, 4 Suppl 1, S4		802
492	Alternative (non-animal) methods for cosmetics testing: current status and future prospects-2010. *Archives of Toxicology*, **2011**, 85, 367-485	5.8	398
491	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. *Environmental Health Perspectives*, **2016**, 124, 1023-33	8.4	206
490	Genotoxicity of metal oxide nanomaterials: review of recent data and discussion of possible mechanisms. *Nanoscale*, **2015**, 7, 2154-98	7.7	135
489	Guidance on the use of the weight of evidence approach in scientific assessments. *EFSA Journal*, **2017**, 15, e04971	2.3	128
488	A European perspective on alternatives to animal testing for environmental hazard identification and risk assessment. *Regulatory Toxicology and Pharmacology*, **2013**, 67, 506-30	3.4	121
487	QSAR as a random event: modeling of nanoparticles uptake in PaCa2 cancer cells. *Chemosphere*, **2013**, 92, 31-7	8.4	114
486	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, 603-13	7.9	107
485	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
484	Interpretation of quantitative structure-property and -activity relationships. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 679-85		100
483	Determination of aromatic amines by solid-phase microextraction and gas chromatography–mass spectrometry in water samples. *Journal of Chromatography A*, **1997**, 791, 221-230	4.5	96
482	In vivo exposure of carp to graded concentrations of bisphenol A. *General and Comparative Endocrinology*, **2007**, 153, 15-24	3	96
481	Automatic knowledge extraction from chemical structures: the case of mutagenicity prediction. *SAR and QSAR in Environmental Research*, **2013**, 24, 365-83	3.5	95
480	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, 1080-7	8.4	92
479	The expanding role of predictive toxicology: an update on the (Q)SAR models for mutagens and carcinogens. *Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews*, **2007**, 25, 53-97	4.5	92
478	Computational predictive programs (expert systems) in toxicology. *Toxicology*, **1997**, 119, 213-25	4.4	86
477	Predictive models for carcinogenicity and mutagenicity: frameworks, state-of-the-art, and perspectives. *Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews*, **2009**, 27, 57-90	4.5	85

476	New public QSAR model for carcinogenicity. *Chemistry Central Journal*, **2010**, 4 Suppl 1, S3		85
475	A new hybrid system of QSAR models for predicting bioconcentration factors (BCF). *Chemosphere*, **2008**, 73, 1701-7	8.4	82
474	CORAL: quantitative structure-activity relationship models for estimating toxicity of organic compounds in rats. *Journal of Computational Chemistry*, **2011**, 32, 2727-33	3.5	80
473	Predicting logP of pesticides using different software. *Chemosphere*, **2003**, 53, 1155-64	8.4	80
472	Novel application of the CORAL software to model cytotoxicity of metal oxide nanoparticles to bacteria Escherichia coli. *Chemosphere*, **2012**, 89, 1098-102	8.4	78
471	Volatile organic compounds produced during the aerobic biological processing of municipal solid waste in a pilot plant. *Chemosphere*, **2005**, 59, 423-30	8.4	72
470	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. *Environmental Health Perspectives*, **2020**, 128, 27002	8.4	70
469	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
468	Comparison of in silico models for prediction of mutagenicity. *Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews*, **2013**, 31, 45-66	4.5	68
467	Estrogenicity profile and estrogenic compounds determined in river sediments by chemical analysis, ELISA and yeast assays. *Chemosphere*, **2008**, 73, 1078-89	8.4	68
466	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. *Environmental Science and Pollution Research*, **2013**, 20, 1649-60	5.1	65
465	Analysis of some pesticides in water samples using solid-phase microextraction-gas chromatography with different mass spectrometric techniques. *Journal of Chromatography A*, **1999**, 859, 193-201	4.5	63
464	Comparison of in silico tools for evaluating rat oral acute toxicity. *SAR and QSAR in Environmental Research*, **2015**, 26, 1-27	3.5	62
463	A generalizable definition of chemical similarity for read-across. *Journal of Cheminformatics*, **2014**, 6, 39	8.6	61
462	Predictive carcinogenicity: a model for aromatic compounds, with nitrogen-containing substituents, based on molecular descriptors using an artificial neural network. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 1076-80		60
461	Automated sample preparation with extraction columns followed by liquid chromatography-ionspray mass spectrometry interferences, determination and degradation of polar organophosphorus pesticides in water samples. *Journal of Chromatography A*, **1996**, 737, 47-58	4.5	59
460	In silico methods to predict drug toxicity. *Current Opinion in Pharmacology*, **2013**, 13, 802-6	5.1	58
459	Sterols in sediment samples from Venice Lagoon, Italy. *Chemosphere*, **1996**, 33, 2383-2393	8.4	58

458	Simultaneous analysis of 50 pesticides in water samples by solid phase extraction and GC-MS. *Chemosphere*, **1990**, 21, 1411-1421	8.4	58
457	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
456	REACH and in silico methods: an attractive opportunity for medicinal chemists. *Drug Discovery Today*, **2014**, 19, 1757-1768	8.8	55
455	Patterns and Sources of Polychlorinated Dibenzo-p-dioxins and Dibenzofurans in Sediments from the Venice Lagoon, Italy. *Environmental Science & Technology*, **1997**, 31, 1777-1784	10.3	53
454	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
453	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
452	Levels of PCDD/F and dioxin-like PCB in Baltic fish of different age and gender. *Chemosphere*, **2008**, 71, 369-78	8.4	49
451	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, 273-98	4.5	48
450	QSAR modeling of Daphnia magna and fish toxicities of biocides using 2D descriptors. *Chemosphere* , **2019**, 229, 8-17	8.4	47
449	PCDD/Fs and PCBs in ambient air in a highly industrialized city in northern Italy. *Chemosphere*, **2013**, 90, 2352-7	8.4	47
448	CORAL: QSAR modeling of toxicity of organic chemicals towards Daphnia magna. *Chemometrics and Intelligent Laboratory Systems*, **2012**, 110, 177-181	3.8	47
447	Investigating the estrogenic risk along the river Po and its intermediate section. *Archives of Environmental Contamination and Toxicology*, **2006**, 51, 641-51	3.2	47
446	Investigating landfill leachate toxicity in vitro: A review of cell models and endpoints. *Environment International*, **2019**, 122, 21-30	12.9	46
445	CORAL: building up the model for bioconcentration factor and defining it's applicability domain. *European Journal of Medicinal Chemistry*, **2011**, 46, 1400-3	6.8	45
444	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	3.5	44
443	Description of the electronic structure of organic chemicals using semiempirical and ab initio methods for development of toxicological QSARs. *Journal of Chemical Information and Modeling*, **2005**, 45, 106-14	6.1	44
442	Validation of counter propagation neural network models for predictive toxicology according to the OECD principles: a case study. *SAR and QSAR in Environmental Research*, **2006**, 17, 265-84	3.5	44
441	Polychlorinated dibenzo-p-dioxins (PCDD) and polychlorinated dibenzofurans (PCDF) in emissions from an urban incineratop. 1. Average and peak values. *Chemosphere*, **1982**, 11, 577-583	8.4	44

440	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
439	SMILES as an alternative to the graph in QSAR modelling of bee toxicity. *Computational Biology and Chemistry*, **2007**, 31, 57-60	3.6	43
438	Additive SMILES-based optimal descriptors in QSAR modelling bee toxicity: Using rare SMILES attributes to define the applicability domain. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 4801-9	3.4	43
437	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
436	Modeling toxicity by using supervised kohonen neural networks. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 485-92		42
435	Assessment and validation of the CAESAR predictive model for bioconcentration factor (BCF) in fish. *Chemistry Central Journal*, **2010**, 4 Suppl 1, S1		41
434	QSAR modeling of measured binding affinity for fullerene-based HIV-1 PR inhibitors by CORAL. *Journal of Mathematical Chemistry*, **2010**, 48, 959-987	2.1	40
433	SMILES in QSPR/QSAR Modeling: results and perspectives. *Current Drug Discovery Technologies*, **2007**, 4, 77-116	1.5	40
432	De novo synthesis of PCDD, PCDF, PCB, PCN and PAH in a pilot incinerator. *Chemosphere*, **1991**, 22, 1045-1052	8.4	40
431	Comparison of SMILES and molecular graphs as the representation of the molecular structure for QSAR analysis for mutagenic potential of polyaromatic amines. *Chemometrics and Intelligent Laboratory Systems*, **2011**, 109, 94-100	3.8	39
430	Binary classification models for endocrine disrupter effects mediated through the estrogen receptor. *SAR and QSAR in Environmental Research*, **2008**, 19, 697-733	3.5	38
429	Increased concentrations of nitrophenols in leaves from a damaged forestal site. *Chemosphere*, **1999**, 38, 1495-1503	8.4	38
428	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
427	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
426	SMILES-based optimal descriptors: QSAR analysis of fullerene-based HIV-1 PR inhibitors by means of balance of correlations. *Journal of Computational Chemistry*, **2010**, 31, 381-92	3.5	37
425	QSAR models for Daphnia toxicity of pesticides based on combinations of topological parameters of molecular structures. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 2779-88	3.4	37
424	Predicting acute contact toxicity of pesticides in honeybees (Apis mellifera) through a k-nearest neighbor model. *Chemosphere*, **2017**, 166, 438-444	8.4	36
423	Quantitative consensus of bioaccumulation models for integrated testing strategies. *Environment International*, **2012**, 45, 51-8	12.9	36

422	Comparison of genistein metabolism in rats and humans using liver microsomes and hepatocytes. *Food and Chemical Toxicology*, **2008**, 46, 939-48	4.7	36
421	QSAR model for predicting pesticide aquatic toxicity. *Journal of Chemical Information and Modeling*, **2005**, 45, 1767-74	6.1	36
420	Comparative studies of the leachate of an industrial landfill by gas chromatography-mass spectrometry, liquid chromatography-nuclear magnetic resonance and liquid chromatography-mass spectrometry. *Journal of Chromatography A*, **1999**, 831, 243-56	4.5	36
419	An alternative QSAR-based approach for predicting the bioconcentration factor for regulatory purposes. *ALTEX: Alternatives To Animal Experimentation*, **2014**, 31, 23-36	4.3	36
418	Ecotoxicological assessment of pharmaceuticals and personal care products using predictive toxicology approaches. *Green Chemistry*, **2020**, 22, 1458-1516	10	36
417	A comparative survey of chemistry-driven in silico methods to identify hazardous substances under REACH. *Regulatory Toxicology and Pharmacology*, **2013**, 66, 301-14	3.4	35
416	SMILES-based optimal descriptors: QSAR modeling of carcinogenicity by balance of correlations with ideal slopes. *European Journal of Medicinal Chemistry*, **2010**, 45, 3581-7	6.8	35
415	GC-MS analysis of dichlobenil and its metabolites in groundwater. *Talanta*, **2005**, 68, 146-54	6.2	35
414	QSAR in ecotoxicity: an overview of modern classification techniques. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 105-12		35
413	The importance of scaling in data mining for toxicity prediction. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 1250-5		35
412	SAR and QSAR modeling of a large collection of LD rat acute oral toxicity data. *Journal of Cheminformatics*, **2019**, 11, 58	8.6	34
411	Meta-analysis of toxicity and teratogenicity of 133 chemicals from zebrafish developmental toxicity studies. *Reproductive Toxicology*, **2013**, 41, 98-108	3.4	34
410	Additive SMILES-based carcinogenicity models: Probabilistic principles in the search for robust predictions. *International Journal of Molecular Sciences*, **2009**, 10, 3106-27	6.3	34
409	A new semi-automated workflow for chemical data retrieval and quality checking for modeling applications. *Journal of Cheminformatics*, **2018**, 10, 60	8.6	34
408	Nano-QSAR: Model of mutagenicity of fullerene as a mathematical function of different conditions. *Ecotoxicology and Environmental Safety*, **2016**, 124, 32-36	7	33
407	Ecotoxicological QSAR modeling of endocrine disruptor chemicals. *Journal of Hazardous Materials*, **2019**, 369, 707-718	12.8	33
406	Optimal nano-descriptors as translators of eclectic data into prediction of the cell membrane damage by means of nano metal-oxides. *Environmental Science and Pollution Research*, **2015**, 22, 745-57	5.1	33
405	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

404	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, 336-44	10.2	33
403	The ToxBank Data Warehouse: Supporting the Replacement of In Vivo Repeated Dose Systemic Toxicity Testing. *Molecular Informatics*, **2013**, 32, 47-63	3.8	33
402	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 and Intelligent Laboratory Systems*, **2011**, 105, 215-219	3.8	33
401	PCDD, PCDF, PCB, PAH, cadmium and lead in roadside soil: relationship between road distance and concentration. *Chemosphere*, **1992**, 24, 1077-1083	8.4	32
400	In silico models for predicting ready biodegradability under REACH: a comparative study. *Science of the Total Environment*, **2013**, 463-464, 161-8	10.2	31
399	QSAR model as a random event: A case of rat toxicity. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 1223-30	3.4	31
398	Evaluation and comparison of benchmark QSAR models to predict a relevant REACH endpoint: The bioconcentration factor (BCF). *Environmental Research*, **2015**, 137, 398-409	7.9	31
397	PCDD/Fs in ambient air in north-east Italy: the role of a MSWI inside an industrial area. *Chemosphere* , **2009**, 77, 1224-9	8.4	31
396	QSAR model for predicting cell viability of human embryonic kidney cells exposed to SiO□ nanoparticles. *Chemosphere*, **2016**, 144, 995-1001	8.4	30
395	Comparison of in silico models for prediction of Daphnia magna acute toxicity. *SAR and QSAR in Environmental Research*, **2014**, 25, 673-94	3.5	30
394	CORAL: QSPR model of water solubility based on local and global SMILES attributes. *Chemosphere*, **2013**, 90, 877-80	8.4	30
393	Combining unsupervised and supervised artificial neural networks to predictaquatic toxicity. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 1897-902		30
392	Factors influencing predictive models for toxicology. *SAR and QSAR in Environmental Research*, **2001**, 12, 593-603	3.5	30
391	coral Software: QSAR for Anticancer Agents. *Chemical Biology and Drug Design*, **2011**, 77, 471-6	2.9	29
390	In silico-aided prediction of biological properties of chemicals: oestrogen receptor-mediated effects. *Chemical Society Reviews*, **2008**, 37, 441-50	58.5	29
389	Directions in QSAR modeling for regulatory uses in OECD member countries, EU and in Russia. *Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews*, **2008**, 26, 201-36	4.5	29
388	Comparative quantitative structure-activity-activity relationships for toxicity to Tetrahymena pyriformis and Pimephales promelas. *ATLA Alternatives To Laboratory Animals*, **2007**, 35, 15-24	2.1	29
387	QSPR modeling for enthalpies of formation of organometallic compounds by means of SMILES-based optimal descriptors. *Chemical Physics Letters*, **2008**, 461, 343-347	2.5	29

386	Involvement of a serine protease in the synthesis of platelet-activating factor by endothelial cells stimulated by tumor necrosis factor-alpha or interleukin-1 alpha. *European Journal of Immunology*, **1994**, 24, 3131-9	6.1	29
385	Screening of 21 pesticides in water by single extraction with C18 silica bonded phase columns and HRGC-MS. *Chemosphere*, **1988**, 17, 59-65	8.4	29
384	Chemometric modeling of Daphnia magna toxicity of agrochemicals. *Chemosphere*, **2019**, 224, 470-479	8.4	28
383	Additive InChI-based optimal descriptors: QSPR modeling of fullerene C 60 solubility in organic solvents. *Journal of Mathematical Chemistry*, **2009**, 46, 1232-1251	2.1	28
382	A new in silico classification model for ready biodegradability, based on molecular fragments. *Chemosphere*, **2014**, 108, 10-6	8.4	27
381	CORAL: QSPR models for solubility of [C60] and [C70] fullerene derivatives. *Molecular Diversity*, **2011**, 15, 249-56	3.1	27
380	A new bioconcentration factor model based on SMILES and indices of presence of atoms. *European Journal of Medicinal Chemistry*, **2010**, 45, 4399-402	6.8	27
379	The proposal of architecture for chemical splitting to optimize QSAR models for aquatic toxicity. *Chemosphere*, **2008**, 72, 772-80	8.4	27
378	Classification of potential endocrine disrupters on the basis of molecular structure using a nonlinear modeling method. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 300-9		27
377	A POLARIZATION FLUORESCENCE IMMUNOASSAY FOR THE HERBICIDE PROPANIL. *Analytical Letters*, **2001**, 34, 2285-2301	2.2	27
376	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
375	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
374	Identification of structural alerts for liver and kidney toxicity using repeated dose toxicity data. *Chemistry Central Journal*, **2015**, 9, 62		26
373	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	1.8	26
372	Metabolites of Alachlor in Water: Identification by Mass Spectrometry and Chemical Synthesis. *Environmental Science & Technology*, **1997**, 31, 3637-3646	10.3	26
371	QSAR models of quail dietary toxicity based on the graph of atomic orbitals. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 1941-3	2.9	26
370	QSAR modelling of aldehyde toxicity by means of optimisation of correlation weights of nearest neighbouring codes. *Computational and Theoretical Chemistry*, **2004**, 676, 165-169		26
369	Emerging organic contaminants in leachates from industrial waste landfills and industrial effluent. *TrAC - Trends in Analytical Chemistry*, **2003**, 22, 757-765	14.6	26

368	VOC exposures in California early childhood education environments. *Indoor Air*, **2017**, 27, 609-621	5.4	25
367	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
366	QSPR modeling bioconcentration factor (BCF) by balance of correlations. *European Journal of Medicinal Chemistry*, **2009**, 44, 2544-51	6.8	25
365	InChI-based optimal descriptors: QSAR analysis of fullerene[C60]-based HIV-1 PR inhibitors by correlation balance. *European Journal of Medicinal Chemistry*, **2010**, 45, 1387-94	6.8	25
364	Predicting toxicity through computers: a changing world. *Chemistry Central Journal*, **2007**, 1, 32		25
363	Virtual screening for aryl hydrocarbon receptor binding prediction. *Journal of Medicinal Chemistry*, **2006**, 49, 5702-9	8.3	25
362	A QSAR Study of Avian Oral Toxicity using Support Vector Machines and Genetic Algorithms. *QSAR and Combinatorial Science*, **2006**, 25, 616-628		25
361	EVALUATION OF SOLID PHASE MICROEXTRACTION□AS CHROMATOGRAPHY IN THE ANALYSIS OF SOME PESTICIDES WITH DIFFERENT MASS SPECTROMETRIC TECHNIQUES: APPLICATION TO ENVIRONMENTAL WATERS AND FOOD SAMPLES. *Analytical Letters*, **2002**, 35, 327-338	2.2	25
360	QSAR models for ACE-inhibitor activity of tri-peptides based on representation of the molecular structure by graph of atomic orbitals and SMILES. *Structural Chemistry*, **2012**, 23, 1873-1878	1.8	24
359	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. *Open Chemistry*, **2011**, 9, 165-174	1.6	24
358	Accelerated solvent extraction then liquid chromatography coupled with mass spectrometry for determination of 4-t-octylphenol, 4-nonylphenols, and bisphenol A in fish liver. *Chromatographia*, **2002**, 56, 463-467	2.1	24
357	Molecular species analysis of phospholipids by negative ion fast atom bombardment mass spectrometry: application of surface precipitation technique. *Biomedical & Environmental Mass Spectrometry*, **1989**, 18, 1051-6		24
356	Physicochemical and analytical characteristics of amiodarone. *Journal of Pharmaceutical Sciences*, **1984**, 73, 829-31	3.9	24
355	Chemical characterization and ecotoxicity of three soil foaming agents used in mechanized tunneling. *Journal of Hazardous Materials*, **2015**, 296, 210-220	12.8	23
354	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
353	Polychlorinated dibenzo-p-dioxins and dibenzofurans in River Po sediments. *Chemosphere*, **2002**, 49, 749-54	8.4	23
352	Fractionation and toxicity evaluation of waste waters. *Journal of Chromatography A*, **2000**, 889, 149-54	4.5	23
351	Identification of an acidic metabolite of N-nitrosodiethanolamine isolated from rat urine. *Biomedical Mass Spectrometry*, **1983**, 10, 334-7		23

350	Polychlorinated dibenzo-p-dioxins (PCDD) and polychlorinated dibenzofurans (PCDF) in emissions from an urban incinerator. 2. Correlation between concentration of micropollutants and combustion conditions. *Chemosphere*, **1983**, 12, 1151-1157	8.4	23
349	Integrating in silico models to enhance predictivity for developmental toxicity. *Toxicology*, **2016**, 370, 127-137	4.4	23
348	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
347	Integrated in silico strategy for PBT assessment and prioritization under REACH. *Environmental Research*, **2016**, 151, 478-492	7.9	22
346	Optimal descriptor as a translator of eclectic information into the prediction of membrane damage: the case of a group of ZnO and TiO2 nanoparticles. *Ecotoxicology and Environmental Safety*, **2014**, 108, 203-9	7	22
345	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	3.5	22
344	Concentrations of PCDD/PCDF in soil close to a secondary aluminum smelter. *Chemosphere*, **2011**, 85, 1719-24	8.4	22
343	Comparison and possible use of in silico tools for carcinogenicity within REACH legislation. *Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews* , **2011**, 29, 300-23	4.5	22
342	Correlation weighting of valence shells in QSAR analysis of toxicity. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 3923-8	3.4	22
341	A GC-MS method for the analysis of fecal and plant sterols in sediment samples. *Chemosphere*, **1994** , 29, 1393-1405	8.4	22
340	Green Chemistry in the Synthesis of Pharmaceuticals.. *Chemical Reviews*, **2021**,	68.1	22
339	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
338	Docking-based classification models for exploratory toxicology studies on high-quality estrogenic experimental data. *Future Medicinal Chemistry*, **2015**, 7, 1921-36	4.1	21
337	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
336	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	10.2	21
335	CORAL: Models of toxicity of binary mixtures. *Chemometrics and Intelligent Laboratory Systems*, **2012**, 119, 39-43	3.8	21
334	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, 974-82	2.2	21
333	Optimisation of correlation weights of SMILES invariants for modelling oral quail toxicity. *European Journal of Medicinal Chemistry*, **2007**, 42, 606-13	6.8	21

332	Tuning neural and fuzzy-neural networks for toxicity modeling. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 513-8		21
331	Concentrations of PCDD and PCDF in different points of a modern refuse incinerator. *Chemosphere*, **1990**, 21, 507-517	8.4	21
330	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
329	CORAL: Predictions of rate constants of hydroxyl radical reaction using representation of the molecular structure obtained by combination of SMILES and Graph approaches. *Chemometrics and Intelligent Laboratory Systems*, **2012**, 112, 65-70	3.8	20
328	Comparing in vivo, in vitro and in silico methods and integrated strategies for chemical assessment: problems and prospects. *ATLA Alternatives To Laboratory Animals*, **2010**, 38, 153-66	2.1	20
327	The CAESAR project for in silico models for the REACH legislation. *Chemistry Central Journal*, **2010**, 4 Suppl 1, I1		20
326	Top-priority fragment QSAR approach in predicting pesticide aquatic toxicity. *Chemical Research in Toxicology*, **2006**, 19, 1533-9	4	20
325	Analysis of chlorinated 1,3-butadienes by solid-phase microextraction and gas chromatography-mass spectrometry. *Journal of Chromatography A*, **1996**, 737, 85-91	4.5	20
324	Using toxicological evidence from QSAR models in practice. *ALTEX: Alternatives To Animal Experimentation*, **2013**, 30, 19-40	4.3	20
323	New Quantitative Structure-Activity Relationship Models Improve Predictability of Ames Mutagenicity for Aromatic Azo Compounds. *Toxicological Sciences*, **2016**, 153, 316-26	4.4	19
322	The definition of the molecular structure for potential anti-malaria agents by the Monte Carlo method. *Structural Chemistry*, **2013**, 24, 1369-1381	1.8	19
321	Integration of QSAR models for bioconcentration suitable for REACH. *Science of the Total Environment*, **2013**, 456-457, 325-32	10.2	19
320	Analysis of organic micropollutants in sediment samples of the Venice Lagoon, Italy. *Water, Air, and Soil Pollution*, **1997**, 99, 237-244	2.6	19
319	Regulatory perspectives in the use and validation of QSAR. A case study: DEMETRA model for Daphnia toxicity. *Environmental Science & Technology*, **2008**, 42, 491-6	10.3	19
318	A protocol to select high quality datasets of ecotoxicity values for pesticides. *Journal of Environmental Science and Health - Part B Pesticides, Food Contaminants, and Agricultural Wastes*, **2004**, 39, 641-52	2.2	19
317	Dictyostelium cells produce platelet-activating factor in response to cAMP. *FEBS Journal*, **1991**, 196, 609-15		19
316	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	8.4	19
315	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

314	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
313	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
312	QSAR modelling of carcinogenicity by balance of correlations. *Molecular Diversity*, **2009**, 13, 367-73	3.1	18
311	An automated group contribution method in predicting aquatic toxicity: the diatomic fragment approach. *Chemical Research in Toxicology*, **2005**, 18, 740-6	4	18
310	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. *Journal of Medicinal Chemistry*, **2005**, 48, 7628-36	8.3	18
309	Identification of organic contaminants in leachates from industrial waste landfills. *TrAC - Trends in Analytical Chemistry*, **1996**, 15, 305-310	14.6	18
308	Synthesis and destruction of PCDD and PCDF inside a municipal solid waste incinerator. *Chemosphere*, **1991**, 23, 715-722	8.4	18
307	Migration of vinyl chloride into PVC-bottled drinking-water assessed by gas chromatography-mass spectrometry. *Food and Chemical Toxicology*, **1991**, 29, 131-4	4.7	18
306	Quasi-SMILES as a tool to utilize eclectic data for predicting the behavior of nanomaterials. *NanoImpact*, **2016**, 1, 60-64	5.6	18
305	Could deep learning in neural networks improve the QSAR models?. *SAR and QSAR in Environmental Research*, **2019**, 30, 617-642	3.5	17
304	Evaluation of QSAR models for predicting the partition coefficient (log P) of chemicals under the REACH regulation. *Environmental Research*, **2015**, 143, 26-32	7.9	17
303	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
302	QSAR model for cytotoxicity of SiO2 nanoparticles on human lung fibroblasts. *Journal of Nanoparticle Research*, **2014**, 16, 1	2.3	17
301	Immunofluorescence detection and localization of B[a]P and TCDD in earthworm tissues. *Chemosphere*, **2014**, 107, 282-289	8.4	17
300	CORAL: QSAR models for acute toxicity in fathead minnow (Pimephales promelas). *Journal of Computational Chemistry*, **2012**, 33, 1218-23	3.5	17
299	CORAL: Monte Carlo Method as a Tool for the Prediction of the Bioconcentration Factor of Industrial Pollutants. *Molecular Informatics*, **2013**, 32, 145-54	3.8	17
298	Simplified molecular input line entry system-based optimal descriptors: quantitative structure-activity relationship modeling mutagenicity of nitrated polycyclic aromatic hydrocarbons. *Chemical Biology and Drug Design*, **2009**, 73, 515-25	2.9	17
297	Endocrine modulation, inhibition of ovarian development and hepatic alterations in rainbow trout exposed to polluted river water. *Environmental Pollution*, **2010**, 158, 3675-83	9.3	17

296	Definition and detection of outliers in chemical space. *Journal of Chemical Information and Modeling* , **2008**, 48, 1592-601	6.1	17
295	QSAR modelling of aldehyde toxicity against a protozoan, Tetrahymena pyriformis by optimization of correlation weights of nearest neighboring codes. *Computational and Theoretical Chemistry*, **2004**, 679, 225-228		17
294	Predicting Toxicity against the fathead Minnow by Adaptive Fuzzy Partition. *QSAR and Combinatorial Science*, **2003**, 22, 210-219		17
293	Alachlor and its metabolites in surface water. *Chemosphere*, **1996**, 32, 229-237	8.4	17
292	Urinary excretion of platelet activating factor in patients with immune-mediated glomerulonephritis. *Kidney International*, **1993**, 43, 426-9	9.9	17
291	Results of a round-robin exercise on read-across. *SAR and QSAR in Environmental Research*, **2016**, 27, 371-84	3.5	17
290	Development, validation and integration of in silico models to identify androgen active chemicals. *Chemosphere*, **2019**, 220, 204-215	8.4	17
289	Towards a systematic use of effect biomarkers in population and occupational biomonitoring. *Environment International*, **2021**, 146, 106257	12.9	17
288	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
287	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
286	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
285	QSAR models for toxicity of organic substances to Daphnia magna built up by using the CORAL freeware. *Chemical Biology and Drug Design*, **2012**, 79, 332-8	2.9	16
284	Toxicological evaluation of urban waste incinerator emissions. *Chemosphere*, **1983**, 12, 559-564	8.4	16
283	A comparison of three methods of soft ionization mass spectrometry of crude phospholipid extracts. *Biological Mass Spectrometry*, **1985**, 12, 643-51		16
282	Metabolic studies of a podophyllotoxin derivative (VP16) in the isolated perfused liver. *Xenobiotica*, **1985**, 15, 343-50	2	16
281	Exploring QSAR modeling of toxicity of chemicals on earthworm. *Ecotoxicology and Environmental Safety*, **2020**, 190, 110067	7	16
280	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
279	Phytotoxicity of wear debris from traditional and innovative brake pads. *Environment International*, **2019**, 123, 156-163	12.9	16

278	CORAL: model for no observed adverse effect level (NOAEL). *Molecular Diversity*, **2015**, 19, 563-75	3.1	15
277	Comparison between bioconcentration factor (BCF) data provided by industry to the European Chemicals Agency (ECHA) and data derived from QSAR models. *Environmental Research*, **2015**, 142, 529-34	3.9	15
276	Integrating QSAR and read-across for environmental assessment. *SAR and QSAR in Environmental Research*, **2015**, 26, 605-18	3.5	15
275	CORAL: prediction of binding affinity and efficacy of thyroid hormone receptor ligands. *European Journal of Medicinal Chemistry*, **2015**, 101, 452-61	6.8	15
274	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
273	CORAL: Building up QSAR models for the chromosome aberration test. *Saudi Journal of Biological Sciences*, **2019**, 26, 1101-1106	4	15
272	Assessment of in silico models for acute aquatic toxicity towards fish under REACH regulation. *SAR and QSAR in Environmental Research*, **2015**, 26, 977-999	3.5	15
271	QSAR-modeling of toxicity of organometallic compounds by means of the balance of correlations for InChI-based optimal descriptors. *Molecular Diversity*, **2010**, 14, 183-92	3.1	15
270	QSAR models for Daphnia magna toxicity prediction of benzoxazinone allelochemicals and their transformation products. *Journal of Agricultural and Food Chemistry*, **2006**, 54, 1111-5	5.7	15
269	Predictive models for aquatic toxicity of aldehydes designed for various model chemistries. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 976-84		15
268	Polychlorinated dibenzo-p-dioxins and dibenzofurans in the air of Seveso, Italy, 26 years after the explosion. *Environmental Science & Technology*, **2003**, 37, 1503-8	10.3	15
267	(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
266	Soil quality in the Lomellina area using in vitro models and ecotoxicological assays. *Environmental Research*, **2014**, 133, 220-31	7.9	14
265	Evaluating the applicability domain in the case of classification predictive models for carcinogenicity based on the counter propagation artificial neural network. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 1147-58	4.2	14
264	Assessing the environmental risks associated with contaminated sites: Definition of an Ecotoxicological Classification index for landfill areas (ECRIS). *Chemosphere*, **2010**, 80, 60-6	8.4	14
263	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. *Journal of Chemical Information and Modeling*, **2005**, 45, 634-44	6.1	14
262	Reaction of 2-amino-2-deoxy-D-glucose and lysine: isolation and characterization of 2,5-bis(tetrahydroxybutyl)pyrazine. *Carbohydrate Research*, **1988**, 184, 67-75	2.9	14
261	Identification and quantitation of 1-arylpiperazines, metabolites resulting from side-chain cleavage of (4-substituted aryl-1-piperazinyl)alkyl heterocyclic derivatives in rat plasma and brain. *Journal of Chromatography A*, **1984**, 283, 211-21	4.5	14

260	First report on a classification-based QSAR model for chemical toxicity to earthworm. *Journal of Hazardous Materials*, **2020**, 386, 121660	12.8	14
259	CATMoS: Collaborative Acute Toxicity Modeling Suite. *Environmental Health Perspectives*, **2021**, 129, 47013	8.4	14
258	QSAR modelling toxicity toward rats of inorganic substances by means of CORAL. *Open Chemistry*, **2011**, 9, 75-85	1.6	13
257	QSAR model for the prediction of bio-concentration factor using aqueous solubility and descriptors considering various electronic effects. *SAR and QSAR in Environmental Research*, **2010**, 21, 711-29	3.5	13
256	QSPR modeling of octanol water partition coefficient of platinum complexes by InChI-based optimal descriptors. *Journal of Mathematical Chemistry*, **2009**, 46, 1060-1073	2.1	13
255	QSPR modeling of octanol/water partition coefficient of antineoplastic agents by balance of correlations. *European Journal of Medicinal Chemistry*, **2010**, 45, 1639-47	6.8	13
254	QSAR modelling of the toxicity to Tetrahymena pyriformis by balance of correlations. *Molecular Diversity*, **2010**, 14, 821-7	3.1	13
253	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. *Molecular Diversity*, **2007**, 11, 171-81	3.1	13
252	A combination of 3D-QSAR, docking, local-binding energy (LBE) and GRID study of the species differences in the carcinogenicity of benzene derivatives chemicals. *Journal of Molecular Graphics and Modelling*, **2008**, 27, 147-60	2.8	13
251	Ecotoxicity prediction by adaptive fuzzy partitioning: comparing descriptors computed on 2D and 3D structures. *SAR and QSAR in Environmental Research*, **2006**, 17, 225-51	3.5	13
250	Increased urinary excretion of platelet activating factor in mice with lupus nephritis. *Life Sciences*, **1991**, 48, 1429-37	6.8	13
249	Grid Computing for the Estimation of Toxicity: Acute Toxicity on Fathead Minnow (Pimephales promelas) **2007**, 60-74		13
248	The index of ideality of correlation: models for flammability of binary liquid mixtures. *Chemical Papers*, **2020**, 74, 601-609	1.9	13
247	Physiologically based pharmacokinetic modeling of perfluoroalkyl substances in the human body. *Toxicological and Environmental Chemistry*, **2015**, 97, 814-827	1.4	12
246	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
245	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
244	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
243	Validation of quantitative structure-activity relationship models to predict water-solubility of organic compounds. *Science of the Total Environment*, **2013**, 463-464, 781-9	10.2	12

242	Application of ERICA index to evaluation of soil ecosystem health according to sustainability threshold for chemical impact. *Science of the Total Environment*, **2013**, 443, 134-42	10.2	12
241	ERICA: A multiparametric toxicological risk index for the assessment of environmental healthiness. *Environment International*, **2010**, 36, 665-74	12.9	12
240	CORAL: binary classifications (active/inactive) for Liver-Related Adverse Effects of Drugs. *Current Drug Safety*, **2012**, 7, 257-61	1.4	12
239	Deuterated internal standards for gas chromatographic-mass spectrometric analysis of polar organophosphorus pesticides in water samples. *Journal of Chromatography A*, **1998**, 822, 91-9	4.5	12
238	Toxicity study of allelochemical-like pesticides by a combination of 3D-QSAR, docking, Local Binding Energy (LBE) and GRID approaches. *SAR and QSAR in Environmental Research*, **2007**, 18, 675-92	3.5	12
237	Database mining with adaptive fuzzy partition: Application to the prediction of pesticide toxicity on rats. *Environmental Toxicology and Chemistry*, **2003**, 22, 983-991	3.8	12
236	High-performance liquid chromatographic separation and mass spectrometric identification of propafenone, 5-hydroxypropafenone and N-depropylpropafenone. *Biomedical Applications*, **1988**, 424, 211-4		12
235	Combining Classifiers of Pesticides Toxicity through a Neuro-fuzzy Approach. *Lecture Notes in Computer Science*, **2002**, 293-303	0.9	12
234	Air quality in the Olona Valley and in vitro human health effects. *Science of the Total Environment*, **2017**, 579, 1929-1939	10.2	11
233	Performance of In Silico Models for Mutagenicity Prediction of Food Contact Materials. *Toxicological Sciences*, **2018**, 163, 632-638	4.4	11
232	QSAR modelling for mutagenic potency of heteroaromatic amines by optimal SMILES-based descriptors. *Chemical Biology and Drug Design*, **2009**, 73, 301-12	2.9	11
231	Harmonised pesticide risk trend indicator for food (HAPERITIF): The methodological approach. *Pest Management Science*, **2006**, 62, 1168-76	4.6	11
230	A case study of indoor pollution by Chinese cooking. *Toxicological and Environmental Chemistry*, **1998**, 65, 217-224	1.4	11
229	Selective sulfur oxygenation in phosphoroamidate, thionophosphate, and thiophosphate agrochemicals by perfluoro-cis-2,3-dialkyloxaziridine. *Tetrahedron*, **1995**, 51, 7981-7992	2.4	11
228	Identification of a nitrosamino aldehyde and a nitrosamino acid resulting from beta-oxidation of N-nitrosodiethanolamine. *Chemico-Biological Interactions*, **1984**, 51, 103-13	5	11
227	Kinetics of 3-tert-butyl-4-hydroxyanisole (BHA) in man. *Food and Chemical Toxicology*, **1984**, 22, 901-4	4.7	11
226	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
225	CORAL: Model for octanol/water partition coefficient. *Fluid Phase Equilibria*, **2015**, 397, 44-49	2.5	10

224	QSAR models for inhibitors of physiological impact of Escherichia coli that leads to diarrhea. *Biochemical and Biophysical Research Communications*, **2013**, 432, 214-25	3.4	10
223	**2011**,		10
222	MULTICLASS CLASSIFIER FROM A COMBINATION OF LOCAL EXPERTS: TOWARD DISTRIBUTED COMPUTATION FOR REAL-PROBLEM CLASSIFIERS. *International Journal of Pattern Recognition and Artificial Intelligence*, **2004**, 18, 801-817	1.1	10
221	Organic tracers identification as a convenient strategy in industrial landfills monitoring. *Chemosphere*, **2003**, 51, 677-83	8.4	10
220	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	8.4	10
219	Studies on the tetrachlorodibenzo-p-dioxins (TCDD) and tetrachlorodibenzofurans (TCDF) emitted from an urban incinerator. *Chemosphere*, **1986**, 15, 557-561	8.4	10
218	Safer chemicals using less animals: kick-off of the European ONTOX project. *Toxicology*, **2021**, 458, 152846	4.4	10
217	Nano-QSAR Model for Predicting Cell Viability of Human Embryonic Kidney Cells. *Methods in Molecular Biology*, **2017**, 1601, 275-290	1.4	9
216	Fragment Prioritization on a Large Mutagenicity Dataset. *Molecular Informatics*, **2017**, 36, 1600133	3.8	9
215	Methodology of aiQSAR: a group-specific approach to QSAR modelling. *Journal of Cheminformatics*, **2019**, 11, 27	8.6	9
214	In Silico Methods for Carcinogenicity Assessment. *Methods in Molecular Biology*, **2016**, 1425, 107-19	1.4	9
213	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
212	Optimizing the aquatic toxicity assessment under REACH through an integrated testing strategy (ITS). *Environmental Research*, **2014**, 135, 156-64	7.9	9
211	Optimal descriptor as a translator of eclectic information into the prediction of thermal conductivity of micro-electro-mechanical systems. *Journal of Mathematical Chemistry*, **2013**, 51, 2230-2237	2.1	9
210	Genistein and dicarboximide fungicides in infant formulae from the EU market. *Food Chemistry*, **2013**, 136, 116-9	8.5	9
209	QSPR modeling of enthalpies of formation for organometallic compounds by SMART-based optimal descriptors. *Journal of Computational Chemistry*, **2009**, 30, 2576-82	3.5	9
208	QSAR analysis of 1,4-dihydro-4-oxo-1-(2-thiazolyl)-1,8-naphthyridines exhibiting anticancer activity by optimal SMILES-based descriptors. *Journal of Mathematical Chemistry*, **2010**, 47, 647-666	2.1	9
207	Preliminary analysis of toxicity of benzoxazinones and their metabolites for Folsomia Candida. *Journal of Agricultural and Food Chemistry*, **2006**, 54, 1099-104	5.7	9

206	Chemical analysis, distributed modelling and risk indices. Three fundamental pillars in Risk Assessment. *Scientific World Journal, The*, **2002**, 2, 1617-25	2.2	9
205	Detection and quanification of trihalomethanes in drinking water from Alexandria, Egypt. *Bulletin of Environmental Contamination and Toxicology*, **1996**, 56, 397-404	2.7	9
204	Metabolism of the anticancer agent 1-(4-acetylphenyl)-3,3-dimethyltriazene. *Biomedical Mass Spectrometry*, **1983**, 10, 485-8		9
203	Horseradish peroxidase/hydrogen peroxide-catalyzed oxidation of VP16-213. Identification of a new metabolite. *Chemico-Biological Interactions*, **1985**, 55, 215-24	5	9
202	Calculation of molecular features with apparent impact on both activity of mutagens and activity of anticancer agents. *Anti-Cancer Agents in Medicinal Chemistry*, **2012**, 12, 807-17	2.2	9
201	QSAR Model for Cytotoxicity of Silica Nanoparticles on Human Embryonic Kidney Cells1. *Materials Today: Proceedings*, **2016**, 3, 847-854	1.4	9
200	Chemometric modeling to predict air half-life of persistent organic pollutants (POPs). *Journal of Hazardous Materials*, **2020**, 382, 121035	12.8	9
199	CORAL: Predictive models for cytotoxicity of functionalized nanozeolites based on quasi-SMILES. *Chemosphere*, **2018**, 210, 52-56	8.4	9
198	QSAR Development for Plasma Protein Binding: Influence of the Ionization State. *Pharmaceutical Research*, **2018**, 36, 28	4.5	8
197	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
196	Mutagenicity, anticancer activity and blood brain barrier: similarity and dissimilarity of molecular alerts. *Toxicology Mechanisms and Methods*, **2018**, 28, 321-327	3.6	8
195	Odor threshold prediction by means of the Monte Carlo method. *Ecotoxicology and Environmental Safety*, **2016**, 133, 390-4	7	8
194	(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
193	SMILES-based optimal descriptors: QSAR modeling of estrogen receptor binding affinity by correlation balance. *Structural Chemistry*, **2012**, 23, 529-544	1.8	8
192	Developing innovative in silico models with EFSA's OpenFoodTox database. *EFSA Supporting Publications*, **2017**, 14, 1206E	1.1	8
191	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	3.5	8
190	Simplified molecular input-line entry system and International Chemical Identifier in the QSAR analysis of styrylquinoline derivatives as HIV-1 integrase inhibitors. *Chemical Biology and Drug Design*, **2011**, 77, 343-60	2.9	8
189	Industrial pollutants in ground waters from northern Milan. *Chemosphere*, **1998**, 36, 2007-17	8.4	8

188	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. *International Journal of Environmental Analytical Chemistry*, **1996**, 65, 69-82	1.8	8
187	Batch square-wave voltammetric and flow-injection amperometric determination of trace amounts of bromofenoxim. *Analytica Chimica Acta*, **1995**, 310, 153-160	6.6	8
186	Development of a mass spectrometric method to quantitate platelet activating factor in mouse urine. *Journal of Lipid Research*, **1989**, 30, 1977-81	6.3	8
185	OCWLGI descriptors: theory and praxis. *Current Computer-Aided Drug Design*, **2013**, 9, 226-32	1.4	8
184	New in silico models to predict in vitro micronucleus induction as marker of genotoxicity. *Journal of Hazardous Materials*, **2020**, 385, 121638	12.8	8
183	QSAR model for pesticides toxicity to Rainbow Trout based on "ideal correlations". *Aquatic Toxicology*, **2020**, 227, 105589	5.1	8
182	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
181	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
180	Use of quasi-SMILES to model biological activity of micelle polymer samples. *Structural Chemistry* , **2018**, 29, 1213-1223	1.8	7
179	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
178	Building up QSAR model for toxicity of psychotropic drugs by the Monte Carlo method. *Structural Chemistry*, **2014**, 25, 1067-1073	1.8	7
177	Use and perceived benefits and barriers of QSAR models for REACH: findings from a questionnaire to stakeholders. *Chemistry Central Journal*, **2012**, 6, 159		7
176	Hybrid toxicology expert system: architecture and implementation of a multi-domain hybrid expert system for toxicology. *Chemometrics and Intelligent Laboratory Systems*, **1998**, 43, 135-145	3.8	7
175	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. *Molecular Diversity*, **2007**, 11, 153-69	3.1	7
174	E-MODELLING: FOUNDATIONS AND CASES FOR APPLYING AI TO LIFE SCIENCES. *International Journal on Artificial Intelligence Tools*, **2007**, 16, 243-268	0.9	7
173	Validation of the models **2007**, 185-199		7
172	Characterization of organic and inorganic pollutants in the Adige river (Italy). *Chemosphere*, **1992**, 25, 1665-1674	8.4	7
171	Incineration of agro-industrial wastes and macro- and micropollutants emission. *Chemosphere*, **1992** , 24, 1545-1551	8.4	7

170	Metabolic profile of atrazine and N-nitrosoatrazine in rat urine. *Bulletin of Environmental Contamination and Toxicology*, **1992**, 48, 701-8	2.7	7
169	Metabolism and pharmacokinetics of p-(3,3-dimethyl-1-triazeno) benzoic acid in M5076 sarcoma-bearing mice. *Cancer Chemotherapy and Pharmacology*, **1989**, 24, 354-8	3.5	7
168	Identification of metabolites of tiropramide in human urine. *Biomedical & Environmental Mass Spectrometry*, **1988**, 15, 205-9		7
167	Effect of butylated hydroxyanisole added in vitro or administered to rats on N,N-dibutylnitrosamine and N-butyl-N-(4-hydroxybutyl)nitrosamine metabolism by post-mitochondrial supernatant of liver homogenates. *Toxicology*, **1988**, 48, 71-80	4.4	7
166	Quantitative analysis of minaprine and some of its metabolites with application to kinetic studies in rats. *Journal of Chromatography A*, **1983**, 259, 141-9	4.5	7
165	A k-NN algorithm for predicting the oral sub-chronic toxicity in the rat. *ALTEX: Alternatives To Animal Experimentation*, **2014**, 31, 423-32	4.3	7
164	Integrated strategy for mutagenicity prediction applied to food contact chemicals. *ALTEX: Alternatives To Animal Experimentation*, **2018**, 35, 169-178	4.3	7
163	Development of a mass spectrometric method to quantitate platelet activating factor in mouse urine.. *Journal of Lipid Research*, **1989**, 30, 1977-1981	6.3	7
162	A fast atom bombardment-mass spectrometric method to quantitate lysophosphatidylserine in rat brain.. *Journal of Lipid Research*, **1989**, 30, 1983-1986	6.3	7
161	SAR for gastro-intestinal absorption and blood-brain barrier permeation of pesticides. *Chemico-Biological Interactions*, **2018**, 290, 1-5	5	7
160	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
159	Ecotoxicological effects of atmospheric particulate produced by braking systems on aquatic and edaphic organisms. *Environment International*, **2020**, 137, 105564	12.9	6
158	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
157	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
156	Ensemble-Based Modeling of Chemical Compounds with Antimalarial Activity. *Current Topics in Medicinal Chemistry*, **2019**, 19, 957-969	3	6
155	In silico model for mutagenicity (Ames test), taking into account metabolism. *Mutagenesis*, **2019**, 34, 41-48	2.8	6
154	CORAL: the prediction of biodegradation of organic compounds with optimal SMILES-based descriptors. *Open Chemistry*, **2012**, 10, 1042-1048	1.6	6
153	CORAL: QSPRs of enthalpies of formation of organometallic compounds. *Journal of Mathematical Chemistry*, **2013**, 51, 1684-1693	2.1	6

152	QSPR modelling of the octanol/water partition coefficient of organometallic substances by optimal SMILES-based descriptors. *Open Chemistry*, **2009**, 7, 846-856	1.6	6
151	Thermodynamic descriptors derived from density functional theory calculations in prediction of aquatic toxicity. *Journal of Chemical Information and Modeling*, **2005**, 45, 379-85	6.1	6
150	Predicting toxicity: a mechanism of action model of chemical mutagenicity. *Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis*, **2001**, 479, 141-71	3.3	6
149	Synthesis and use of pentadeuteroethyl ethofumesate as an internal standard for the determination of ethofumesate and its metabolites in water by gas chromatography-mass spectrometry. *Journal of Chromatography A*, **1994**, 688, 243-250	4.5	6
148	Measurement of vitamin E in premature infants by reversed-phase high-performance liquid chromatography. *Biomedical Applications*, **1989**, 490, 432-8		6
147	A fast atom bombardment-mass spectrometric method to quantitate lysophosphatidylserine in rat brain. *Journal of Lipid Research*, **1989**, 30, 1983-6	6.3	6
146	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 Metabolism and Disposition*, **1995**, 23, 113-8	4	6
145	Automated integration of structural, biological and metabolic similarities to improve read-across. *ALTEX: Alternatives To Animal Experimentation*, **2020**, 37, 469-481	4.3	6
144	CORAL: classification model for predictions of anti-sarcoma activity. *Current Topics in Medicinal Chemistry*, **2012**, 12, 2741-4	3	6
143	QSAR Models for Human Carcinogenicity: An Assessment Based on Oral and Inhalation Slope Factors. *Molecules*, **2020**, 26,	4.8	6
142	QSPR/QSAR Analyses by Means of the CORAL Software. *Advances in Chemical and Materials Engineering Book Series*, **2015**, 560-585	0.2	6
141	Ecosystem ecology: Models for acute toxicity of pesticides towards Daphnia magna. *Environmental Toxicology and Pharmacology*, **2020**, 80, 103459	5.8	6
140	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
139	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
138	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
137	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
136	Prediction of antimicrobial activity of large pool of peptides using quasi-SMILES. *BioSystems*, **2018**, 169-170, 5-12	1.9	6
135	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

134	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
133	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
132	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
131	QSPR modelling of normal boiling points and octanol/water partition coefficient for acyclic and cyclic hydrocarbons using SMILES-based optimal descriptors. *Open Chemistry*, **2010**, 8, 1047-1052	1.6	5
130	Use of the international chemical identifier for constructing QSPR-model of normal boiling points of acyclic carbonyl substances. *Journal of Mathematical Chemistry*, **2010**, 47, 355-369	2.1	5
129	Results of DEMETRA models **2007**, 201-281		5
128	Applications of Flexible Molecular Descriptors in the QSPR/QSAR Study of Heterocyclic Drugs1-38		5
127	Development of an Enzyme-Linked Immunosorbent Assay (ELISA) for the Herbicide Propanil. *International Journal of Environmental Analytical Chemistry*, **2002**, 82, 865-878	1.8	5
126	GC-MS analysis of n-phosphonomethylglycine (glyphosate) samples through derivatization with a perfluoroanhydride and trifluoroethanol: Identification of by-products. *Toxicological and Environmental Chemistry*, **1993**, 38, 225-232	1.4	5
125	Syntheses of deuterated leu-enkephalins and their use as internal standards for the quantification of leu-enkephalin by fast atom bombardment mass spectrometry. *Journal of Labelled Compounds and Radiopharmaceuticals*, **1990**, 28, 411-419	1.9	5
124	QSAR Methods to Screen Endocrine Disruptors. *Nuclear Receptor Research*, **2016**, 3,	1.4	5
123	Pharmaceuticals as Environmental Contaminants: Modelling Distribution and Fate **2001**, 91-102		5
122	Zebrafish AC modelling: (Q)SAR models to predict developmental toxicity in zebrafish embryo. *Ecotoxicology and Environmental Safety*, **2020**, 202, 110936	7	5
121	'Ideal correlations' for the predictive toxicity to. *Toxicology Mechanisms and Methods*, **2020**, 30, 605-610	3.6	5
120	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
119	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
118	Mixing a Symbolic and a Subsymbolic Expert to Improve Carcinogenicity Prediction of Aromatic Compounds. *Lecture Notes in Computer Science*, **2001**, 126-135	0.9	5
117	VEGAHUB for Ecotoxicological QSAR Modeling. *Methods in Pharmacology and Toxicology*, **2020**, 759-787	1.1	5

116	Structures of Endocrine-Disrupting Chemicals Correlate with the Activation of 12 Classic Nuclear Receptors. *Environmental Science & Technology*, **2021**,	10.3	5
115	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
114	New QSAR models to predict chromosome damaging potential based on the in vivo micronucleus test. *Toxicology Letters*, **2020**, 329, 80-84	4.4	4
113	Use of Read-Across Tools. *Methods in Molecular Biology*, **2016**, 1425, 305-22	1.4	4
112	Classification of a Naïve Bayesian Fingerprint model to predict reproductive toxicity. *SAR and QSAR in Environmental Research*, **2018**, 29, 631-645	3.5	4
111	Synthesis, biological evaluation, and docking studies of PAR2-AP-derived pseudopeptides as inhibitors of kallikrein 5 and 6. *Biological Chemistry*, **2015**, 396, 45-52	4.5	4
110	CORAL: Quantitative models for estimating bioconcentration factor of organic compounds. *Chemometrics and Intelligent Laboratory Systems*, **2012**, 118, 70-73	3.8	4
109	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	2.5	4
108	Food contamination control in European new Member States and associated candidate countries: data collected within the SAFEFOODNET project. *Journal of Environmental Science and Health - Part B Pesticides, Food Contaminants, and Agricultural Wastes*, **2009**, 44, 407-14	2.2	4
107	Support vector machines in the prediction of mutagenicity of chemical compounds **2009**,		4
106	Regulatory assessment of chemicals within OECD member countries, EU and in Russia. *Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews*, **2008**, 26, 40-88	4.5	4
105	QSAR trout toxicity models on aromatic pesticides. *Journal of Environmental Science and Health - Part B Pesticides, Food Contaminants, and Agricultural Wastes*, **2008**, 43, 633-637	2.2	4
104	The specificity of the QSAR models for regulatory purposes: the example of the DEMETRA project. *SAR and QSAR in Environmental Research*, **2007**, 18, 209-20	3.5	4
103	ANVAS: artificial neural variables adaptation system for descriptor selection. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 335-46	4.2	4
102	Environmental agent susceptibility assessment using existing and novel biomarkers as rapid noninvasive testing methods. *Annals of the New York Academy of Sciences*, **2005**, 1040, 381-6	6.5	4
101	Impurities Released from Extractive Phases Used in the Analysis of Pesticides. *International Journal of Environmental Analytical Chemistry*, **1995**, 58, 23-30	1.8	4
100	Analysis of bromofenoxim by supercritical fluid chromatography and comparison with an HPLC method. *Toxicological and Environmental Chemistry*, **1995**, 47, 119-128	1.4	4
99	A Library Report on the Analysis of Pesticides Subject to Investigation for the European Communities Commission. *International Journal of Environmental Analytical Chemistry*, **1995**, 58, 31-42	1.8	4

98	Solid-phase extraction coupled with electrochemical detection for the determination of the herbicide bromofenoxim in water samples at low- and sub-microgram l-1 levels. *Analyst, The*, **1996**, 121, 1839-43	5	4
97	Synthesis and use of deuterated fenamiphos and its metabolites as internal standards for mass spectrometric analysis in water. *Journal of Chromatography A*, **1996**, 754, 207-219	4.5	4
96	Pollution of ground and drinking water with volatile organic compounds: Solid-phase microextraction and GC/MS analysis. *Toxicological and Environmental Chemistry*, **1996**, 55, 73-81	1.4	4
95	First report on chemometric modeling of hydrolysis half-lives of organic chemicals. *Environmental Science and Pollution Research*, **2021**, 28, 1627-1642	5.1	4
94	Ecotoxicological QSAR modeling of the acute toxicity of organic compounds to the freshwater crustacean Thamnocephalus platyurus. *Chemosphere*, **2021**, 280, 130652	8.4	4
93	Integrating in silico models for the prediction of mutagenicity (Ames test) of botanical ingredients of cosmetics. *Computational Toxicology*, **2019**, 12, 100108	3.1	3
92	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
91	Maintenance,update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0. *EFSA Supporting Publications*, **2020**, 17, 1822E	1.1	3
90	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
89	QSPR analysis of threshold of odor for the large number of heterogenic chemicals. *Molecular Diversity*, **2018**, 22, 397-403	3.1	3
88	Development of QSAR models for predicting anti-HIV-1 activity using the Monte Carlo method. *Open Chemistry*, **2013**, 11, 371-380	1.6	3
87	1-(o-Methoxyphenyl)piperazine is a metabolite of drugs bearing a methoxyphenylpiperazine side-chain. *Journal of Pharmacy and Pharmacology*, **1987**, 39, 312-3	4.8	3
86	QSAR modeling of anxiolytic activity taking into account the presence of keto- and enol-tautomers by balance of correlations with ideal slopes. *Open Chemistry*, **2011**, 9, 846-854	1.6	3
85	Identification of toxifying and detoxifying moieties for mutagenicity prediction by priority assessment. *Journal of Chemical Information and Modeling*, **2011**, 51, 1564-74	6.1	3
84	A comparison of DEMETRA individual QSARs with an index for evaluation of uncertainty. *Chemosphere*, **2008**, 71, 1845-52	8.4	3
83	QSARs for regulatory purposes: the case for pesticide authorization **2007**, 1-57		3
82	Hybrid systems **2007**, 149-183		3
81	The quality criteria of the DEMETRA models for regulatory purposes **2007**, 283-301		3

80	Modelling Aquatic Toxicity with Advanced Computational Techniques: Procedures to Standardize Data and Compare Models. *Lecture Notes in Computer Science*, **2004**, 235-248	0.9	3
79	Diurnal, weekly and seasonal air concentrations of PCDD and PCDF in an industrial area. *Freseniusd Journal of Analytical Chemistry*, **1994**, 348, 141-143		3
78	Simultaneous determination of isbufylline and its major metabolites in rabbit blood and urine by reversed-phase high-performance liquid chromatography. *Biomedical Applications*, **1991**, 568, 407-18		3
77	High-performance liquid chromatographic assay for the determination of p-(3,3-dimethyl-1-triazeno)benzoic acid in mouse plasma. *Biomedical Applications*, **1985**, 345, 323-31		3
76	Virtual Screening of Anti-Cancer Compounds: Application of Monte Carlo Technique. *Anti-Cancer Agents in Medicinal Chemistry*, **2019**, 19, 148-153	2.2	3
75	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
74	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
73	The self-organizing vector of atom-pairs proportions: use to develop models for melting points. *Structural Chemistry*, **2021**, 32, 967-971	1.8	3
72	Classification nano-SAR modeling of metal oxides nanoparticles genotoxicity based on comet assay data. *Toxicology Letters*, **2016**, 258, S271	4.4	3
71	Paradox of 'ideal correlations': improved model for air half-life of persistent organic pollutants. *Environmental Technology (United Kingdom)*, **2021**, 1-6	2.6	3
70	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
69	Prediction of Biochemical Endpoints by the CORAL Software: Prejudices, Paradoxes, and Results. *Methods in Molecular Biology*, **2018**, 1800, 573-583	1.4	3
68	Database mining with adaptive fuzzy partition: application to the prediction of pesticide toxicity on rats. *Environmental Toxicology and Chemistry*, **2003**, 22, 983-91	3.8	3
67	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
66	Computational Toxicology and Reach **2018**, 245-268		2
65	Quantitative structure□ctivity relationship models for bee toxicity. *Toxicological and Environmental Chemistry*, **2016**, 1-12	1.4	2
64	Novel chemical hazard characterisation approaches. *EFSA Journal*, **2016**, 14, e00506	2.3	2
63	Databases for pesticide ecotoxicity **2007**, 59-81		2

62	A NICI-GC-MS Method to Analyze Endosulfan in Biological Samples. *International Journal of Environmental Analytical Chemistry*, **1995**, 58, 67-72	1.8	2
61	Mass Spectrometric Studies of Flavonoids. *Natural Product Research*, **1994**, 4, 247-254		2
60	Quantification of 4,4?-diaminodiphenylmethane by gas chromatography negative ion chemical lonization mass spectrometry. *Microchemical Journal*, **1992**, 46, 352-359	4.8	2
59	A gas chromatographic mass spectrometric assay for the determination of aphidicolin in plasma of cancer patients. *Journal of Pharmaceutical Sciences*, **1989**, 78, 399-401	3.9	2
58	The system of self-consistent models for vapour pressure. *Chemical Physics Letters*, **2022**, 790, 139354	2.5	2
57	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
56	Development of Monte Carlo Approaches in Support of Environmental Research. *Challenges and Advances in Computational Chemistry and Physics*, **2017**, 453-469	0.7	2
55	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
54	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
53	SpheraCosmolife: a new tool for the risk assessment of cosmetic products. *ALTEX: Alternatives To Animal Experimentation*, **2021**, 38, 565-579	4.3	2
52	Quantitative Structure-Activity Relationship Modeling of the Amplex Ultrared Assay to Predict Thyroperoxidase Inhibitory Activity. *Frontiers in Pharmacology*, **2021**, 12, 713037	5.6	2
51	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
50	Data-driven modeling and prediction of acute toxicity of pesticide residues. *SIGKDD Explorations: Newsletter of the Special Interest Group (SIG) on Knowledge Discovery & Data Mining*, **2006**, 8, 71-79	4.6	1
49	An interlaboratory analysis on labile pesticides. *Toxicological and Environmental Chemistry*, **1998**, 65, 173-184	1.4	1
48	GC Analysis of Some Organochlorine Pesticides using a Brominated Internal Standard. *International Journal of Environmental Analytical Chemistry*, **1995**, 58, 55-66	1.8	1
47	A simple method for determination of N-nitrosamine traces in trifluralin samples by gas chromatography-mass spectrometry. *Toxicological and Environmental Chemistry*, **1994**, 45, 199-204	1.4	1
46	Mass spectrometric identification of urinary and plasma metabolites of 2-(6'-carboxyhexyl)-3-n-hexylcyclohexylamine, a new antiaggregating agent. *European Journal of Drug Metabolism and Pharmacokinetics*, **1992**, 17, 93-101	2.7	1
45	Specific gas chromatography-mass spectrometry analytical method for the determination of cyhexatin in animal feed. *Journal of Chromatography A*, **1992**, 605, 129-33	4.5	1

44	Preliminary survey on 2,3,7,8-TCDD in cellulose-containing consumer products on the italian market. *Chemosphere*, **1993**, 27, 1561-1564	8.4	1
43	Mass spectrometric identification of urinary and plasma metabolites of 9-hydroxy-19,20-bis-nor-prostanoic acid (rosaprostol). *Prostaglandins*, **1988**, 35, 665-84		1
42	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 Metabolism and Disposition*, **1991**, 19, 913-6	4	1
41	Toxicology is IN: in silico, in vitro, integrated testing strategy. *ALTEX: Alternatives To Animal Experimentation*, **2016**, 33, 187-8	4.3	1
40	Analysis of Organic Micropollutants in Sediment Samples of the Venice Lagoon, Italy **1997**, 237-244		1
39	QSAR-Models, Validation, and IIC-Paradox for Drug Toxicity. *International Journal of Quantitative Structure-Property Relationships*, **2020**, 5, 22-43	1.2	1
38	Maintenance, update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0. *EFSA Supporting Publications*, **2021**, 18, 6476E	1.1	1
37	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
36	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
35	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
34	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
33	Patent Toxicity. *Research Policy*, **2022**, 51, 104329	7.5	1
32	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
31	Development of new QSAR models for water, sediment, and soil half-life. *Science of the Total Environment*, **2022**, 156004	10.2	1
30	Value and limitation of structure-based profilers to characterize developmental and reproductive toxicity potential. *Archives of Toxicology*, **2020**, 94, 939-954	5.8	0
29	Semi-correlations as a tool to model for skin sensitization. *Food and Chemical Toxicology*, **2021**, 157, 112580	4.9	0
28	In Silico Methods for Carcinogenicity Assessment.. *Methods in Molecular Biology*, **2022**, 2425, 201-215	1.4	0
27	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

26	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
25	The VEGAHUB Platform: The Philosophy and the Tools.. *ATLA Alternatives To Laboratory Animals*, **2022**, 2611929221090530	2.1	0
24	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
23	Carcinogenicity prediction using the index of ideality of correlation. *SAR and QSAR in Environmental Research*,1-10	3.5	0
22	Toxicological and Ecotoxicological Studies for Additives. *Handbook of Environmental Chemistry*, **2012**, 73-89	0.8	
21	Toxicological Characterization of Waste-Related Products Using Alternative Methods: Three Case Studies. *Handbook of Environmental Chemistry*, **2012**, 171-205	0.8	
20	Computer-aided methodologies to predict endocrine-disrupting potency of chemicals **2009**, 306-321		
19	Environmental and Ecological Toxicology: Computational Risk Assessment625-650		
18	Open Computing Grid for Molecular Sciences1-21		
17	Characterization of chemical structures **2007**, 83-109		
16	Preparation of 4,4?-diaminodiphenylmethane-(2H4) for use as internal standard in the quantification of 4,4?-diaminodiphenylmethane. *Journal of Labelled Compounds and Radiopharmaceuticals*, **1991**, 29, 725-728	1.9	
15	Analysis by fast atom bombardment mass spectrometry of phospholipids from tubuli, glomeruli, and urine of normal rats and rats with acute renal failure. *Biochemical Medicine and Metabolic Biology*, **1992**, 48, 219-26		
14	From Data to Models **2021**, 89-124		
13	Computational Tools for the Assessment and Substitution of Biocidal Active Substances of Ecotoxicological Concern **2021**, 527-546		
12	Skin sensitization quantitative QSAR models based on mechanistic structural alerts.. *Toxicology*, **2022**, 153111	4.4	
11	Identification of microsomal metabolites of spirogermanium. *Anticancer Research*, **1989**, 9, 507-10	2.3	
10	The Tools for Aquatic Toxicology within the VEGAHUB System **2021**, 493-511		
9	Characterization of the Major Browning Derivatives of Lysine with 2-Amino-2-Deoxy-D-Glucose **1990**, 109-114		

8	QSPR/QSAR Analyses by Means of the CORAL Software **2017**, 929-955	
7	QSAR Models for Regulatory Purposes: Experiences and Perspectives **2009**, 183-200	
6	Chapter 10. In Silico Approaches to Screening Dietary Endocrine Disruptors. *Issues in Toxicology*, **2011**, 170-183	0.3
5	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
4	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
3	Using VEGAHUB Within a Weight-of-Evidence Strategy.. *Methods in Molecular Biology*, **2022**, 2425, 479-495	1.4
2	In Silico Models for Developmental Toxicity.. *Methods in Molecular Biology*, **2022**, 2425, 217-240	1.4
1	Modeling the migration of chemicals from food contact materials to food: The MERLIN-expo/SPHERA toolbox. *Food and Chemical Toxicology*, **2022**, 113118	4.7