

Alessandra Roncaglioni

List of Publications by Year in descending order

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72
papers

2,200
citations

218677
26
h-index

243625
44
g-index

76
all docs

76
docs citations

76
times ranked

2037
citing authors

#	ARTICLE	IF	CITATIONS
1	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	6.0	264
2	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
3	New public QSAR model for carcinogenicity. Chemistry Central Journal, 2010, 4, S3.	2.6	105
4	Predicting logP of pesticides using different software. Chemosphere, 2003, 53, 1155-1164.	8.2	94
5	A new hybrid system of QSAR models for predicting bioconcentration factors (BCF). Chemosphere, 2008, 73, 1701-1707.	8.2	92
6	Comparison of <i>in silico</i> tools for evaluating rat oral acute toxicity. SAR and QSAR in Environmental Research, 2015, 26, 1-27.	2.2	87
7	In silico methods to predict drug toxicity. Current Opinion in Pharmacology, 2013, 13, 802-806.	3.5	72
8	SAR and QSAR modeling of a large collection of LD50 rat acute oral toxicity data. Journal of Cheminformatics, 2019, 11, 58.	6.1	71
9	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
10	Variable Selection and Interpretation in Structure~Affinity Correlation Modeling of Estrogen Receptor Binders. Journal of Chemical Information and Modeling, 2005, 45, 1507-1519.	5.4	61
11	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.	5.4	61
12	CORAL: Building up the model for bioconcentration factor and defining its applicability domain. European Journal of Medicinal Chemistry, 2011, 46, 1400-1403.	5.5	57
13	Evaluation of QSAR Models for the Prediction of Ames Genotoxicity: A Retrospective Exercise on the Chemical Substances Registered Under the EU REACH Regulation. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2014, 32, 273-298.	2.9	57
14	Assessment and validation of the CAESAR predictive model for bioconcentration factor (BCF) in fish. Chemistry Central Journal, 2010, 4, S1.	2.6	54
15	Global QSAR models of skin sensitizers for regulatory purposes. Chemistry Central Journal, 2010, 4, S5.	2.6	51
16	Binary classification models for endocrine disrupter effects mediated through the estrogen receptor. SAR and QSAR in Environmental Research, 2008, 19, 697-733.	2.2	43
17	A comparative survey of chemistry-driven in silico methods to identify hazardous substances under REACH. Regulatory Toxicology and Pharmacology, 2013, 66, 301-314.	2.7	42
18	Evaluation and comparison of benchmark QSAR models to predict a relevant REACH endpoint: The bioconcentration factor (BCF). Environmental Research, 2015, 137, 398-409.	7.5	42

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19	Quantitative consensus of bioaccumulation models for integrated testing strategies. <i>Environment International</i> , 2012, 45, 51-58.	10.0	41
20	Integrating in silico models to enhance predictivity for developmental toxicity. <i>Toxicology</i> , 2016, 370, 127-137.	4.2	39
21	EFSA's OpenFoodTox: An open source toxicological database on chemicals in food and feed and its future developments. <i>Environment International</i> , 2021, 146, 106293.	10.0	36
22	In silico-aided prediction of biological properties of chemicals: oestrogen receptor-mediated effects. <i>Chemical Society Reviews</i> , 2008, 37, 441-450.	38.1	33
23	Factors Influencing Predictive Models for Toxicology. <i>SAR and QSAR in Environmental Research</i> , 2001, 12, 593-603.	2.2	32
24	Integrated in silico strategy for PBT assessment and prioritization under REACH. <i>Environmental Research</i> , 2016, 151, 478-492.	7.5	32
25	Classification of Potential Endocrine Disrupters on the Basis of Molecular Structure Using a Nonlinear Modeling Method. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 300-309.	2.8	29
26	A new bioconcentration factor model based on SMILES and indices of presence of atoms. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 4399-4402.	5.5	29
27	Comparison and Possible Use of In Silico Tools for Carcinogenicity Within REACH Legislation. <i>Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews</i> , 2011, 29, 300-323.	2.9	24
28	New clues on carcinogenicity-related substructures derived from mining two large datasets of chemical compounds. <i>Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews</i> , 2016, 34, 97-113.	2.9	24
29	Coral: QSAR models for acute toxicity in fathead minnow (<i>Pimephales promelas</i>). <i>Journal of Computational Chemistry</i> , 2012, 33, 1218-1223.	3.3	23
30	Development, validation and integration of in silico models to identify androgen active chemicals. <i>Chemosphere</i> , 2019, 220, 204-215.	8.2	23
31	Integrating QSAR models predicting acute contact toxicity and mode of action profiling in honey bees (<i>A. mellifera</i>): Data curation using open source databases, performance testing and validation. <i>Science of the Total Environment</i> , 2020, 735, 139243.	8.0	22
32	Identification of the Structural Requirements of the Receptor-Binding Affinity of Diphenolic Azoles to Estrogen Receptors E_{1} and E_{2} by Three-Dimensional Quantitative Structure-Activity Relationship Analysis. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 7628-7636.	6.4	21
33	Regulatory Perspectives in the Use and Validation of QSAR. A Case Study: DEMETRA Model for <i>Daphnia</i> Toxicity. <i>Environmental Science & Technology</i> , 2008, 42, 491-496.	10.0	21
34	A large comparison of integrated SAR/QSAR models of the Ames test for mutagenicity. <i>SAR and QSAR in Environmental Research</i> , 2018, 29, 591-611.	2.2	21
35	A Protocol to Select High Quality Datasets of Ecotoxicity Values for Pesticides. <i>Journal of Environmental Science and Health - Part B Pesticides, Food Contaminants, and Agricultural Wastes</i> , 2004, 39, 641-652.	1.5	19
36	QSAR model for the prediction of bio-concentration factor using aqueous solubility and descriptors considering various electronic effects. <i>SAR and QSAR in Environmental Research</i> , 2010, 21, 711-729.	2.2	18

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37	Integrating QSAR and read-across for environmental assessment. SAR and QSAR in Environmental Research, 2015, 26, 605-618.	2.2	17
38	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, 1147-1158.	2.9	16
39	Integrated testing strategy (ITS) for bioaccumulation assessment under REACH. Environment International, 2014, 69, 40-50.	10.0	14
40	Ecotoxicity prediction by adaptive fuzzy partitioning: comparing descriptors computed on 2D and 3D structures. SAR and QSAR in Environmental Research, 2006, 17, 225-251.	2.2	13
41	QSAR Models for Human Carcinogenicity: An Assessment Based on Oral and Inhalation Slope Factors. Molecules, 2021, 26, 127.	3.8	13
42	Optimizing the aquatic toxicity assessment under REACH through an integrated testing strategy (ITS). Environmental Research, 2014, 135, 156-164.	7.5	11
43	QSAR Development for Plasma Protein Binding: Influence of the Ionization State. Pharmaceutical Research, 2019, 36, 28.	3.5	11
44	Integrating QSAR, Read-Across, and Screening Tools: The VEGA HUB Platform as an Example. Challenges and Advances in Computational Chemistry and Physics, 2019, , 365-381.	0.6	11
45	In silico model for mutagenicity (Ames test), taking into account metabolism. Mutagenesis, 2019, 34, 41-48.	2.6	10
46	Integrating in silico models for the prediction of mutagenicity (Ames test) of botanical ingredients of cosmetics. Computational Toxicology, 2019, 12, 100108.	3.3	10
47	Automated Integration of Structural, Biological and Metabolic Similarities to Sustain Read-Across. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 469-481.	1.5	10
48	Evaluating confidence in toxicity assessments based on experimental data and in silico predictions. Computational Toxicology, 2022, 21, 100204.	3.3	10
49	The VEGA HUB Platform: The Philosophy and the Tools. ATLA Alternatives To Laboratory Animals, 2022, 50, 121-135.	1.0	10
50	Validation of the models. , 2007, , 185-199.		9
51	<i>In silico</i> tools and transcriptomics analyses in the mutagenicity assessment of cosmetic ingredients: a proof-of-principle on how to add weight to the evidence. Mutagenesis, 2016, 31, 453-461.	2.6	9
52	The system of self-consistent models for vapour pressure. Chemical Physics Letters, 2022, 790, 139354.	2.6	9
53	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, 3053.	4.1	9
54	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.	2.2	8

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55	CORAL: the prediction of biodegradation of organic compounds with optimal SMILES-based descriptors. Open Chemistry, 2012, 10, 1042-1048.	1.9	7
56	In Silico Model for Developmental Toxicity: How to Use QSAR Models and Interpret Their Results. Methods in Molecular Biology, 2016, 1425, 139-161.	0.9	7
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.	2.8	7
58	Results of DEMETRA models. , 2007, , 201-281.		6
59	Prediction of Biochemical Endpoints by the CORAL Software: Prejudices, Paradoxes, and Results. Methods in Molecular Biology, 2018, 1800, 573-583.	0.9	6
60	Principles and procedures for assessment of acute toxicity incorporating in silico methods. Computational Toxicology, 2022, 24, 100237.	3.3	5
61	A comparison of DEMETRA individual QSARs with an index for evaluation of uncertainty. Chemosphere, 2008, 71, 1845-1852.	8.2	4
62	Maintenance, update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0. EFSA Supporting Publications, 2020, 17, 1822E.	0.7	4
63	SpheraCosmolife: a new tool for the risk assessment of cosmetic products. ALTEX: Alternatives To Animal Experimentation, 2021, 38, 565-579.	1.5	4
64	Quantitative Structure-Activity Relationship Modeling of the Amplex Ultrared Assay to Predict Thyroperoxidase Inhibitory Activity. Frontiers in Pharmacology, 2021, 12, 713037.	3.5	4
65	In Silico Methods for Carcinogenicity Assessment. Methods in Molecular Biology, 2022, 2425, 201-215.	0.9	4
66	Carcinogenicity prediction using the index of ideality of correlation. SAR and QSAR in Environmental Research, 2022, 33, 419-428.	2.2	4
67	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.	2.2	3
68	In Silico Models for Developmental Toxicity. Methods in Molecular Biology, 2022, 2425, 217-240.	0.9	3
69	Databases for pesticide ecotoxicity. , 2007, , 59-81.		2
70	Impact of REACH legislation on the production and importation of CMR (carcinogen, mutagen and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Pharmacology, 2019, 101, 166-171.	2.7	1
71	Classification of Potential Endocrine Disrupters on the Basis of Molecular Structure Using a Nonlinear Modeling Method.. ChemInform, 2004, 35, no.	0.0	0
72	Computer-aided methodologies to predict endocrine-disrupting potency of chemicals. , 2009, , 306-321.		0