Alessandra Roncaglioni

List of Publications by Year
in descending order

72	2,200	249298	274796
papers	citations	26 h-index	44 g-index

76	76	76	2225
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Evaluating confidence in toxicity assessments based on experimental data and in silico predictions. Computational Toxicology, 2022, 21, 100204.	1.8	10
2	The system of self-consistent models for vapour pressure. Chemical Physics Letters, 2022, 790, 139354.	1.2	9
3	In Silico Methods for Carcinogenicity Assessment. Methods in Molecular Biology, 2022, 2425, 201-215.	0.4	4
4	In Silico Models for Developmental Toxicity. Methods in Molecular Biology, 2022, 2425, 217-240.	0.4	3
5	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.	1.8	9
6	The VEGAHUB Platform: The Philosophy and the Tools. ATLA Alternatives To Laboratory Animals, 2022, 50, 121-135.	0.7	10
7	Carcinogenicity prediction using the index of ideality of correlation. SAR and QSAR in Environmental Research, 2022, 33, 419-428.	1.0	4
8	Principles and procedures for assessment of acute toxicity incorporating in silico methods. Computational Toxicology, 2022, 24, 100237.	1.8	5
9	EFSAâ€™s OpenFoodTox: An open source toxicological database on chemicals in food and feed and its future developments. Environment International, 2021, 146, 106293.	4.8	36
10	SpheraCosmolife: a new tool for the risk assessment of cosmetic products. ALTEX: Alternatives To Animal Experimentation, 2021, 38, 565-579.	0.9	4
11	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.	1.0	8
12	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	2.8	63
13	Quantitative Structure-Activity Relationship Modeling of the Amplex Ultrared Assay to Predict Thyroperoxidase Inhibitory Activity. Frontiers in Pharmacology, 2021, 12, 713037.	1.6	4
14	QSAR Models for Human Carcinogenicity: An Assessment Based on Oral and Inhalation Slope Factors. Molecules, 2021, 26, 127.	1.7	13
15	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.	1.4	7
16	Evaluation of non-commercial models for genotoxicity and carcinogenicity in the assessment of EFSAâ€™s databases. SAR and QSAR in Environmental Research, 2020, 31, 33-48.	1.0	3
17	Maintenance,update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0. EFSA Supporting Publications, 2020, 17, 1822E.	0.3	4
18	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.	3.9	22

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19	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	2.8	120
20	Automated Integration of Structural, Biological and Metabolic Similarities to Sustain Read-Across. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 469-481.	0.9	10
21	In silico model for mutagenicity (Ames test), taking into account metabolism. Mutagenesis, 2019, 34, 41-48.	1.0	10
22	SAR and QSAR modeling of a large collection of LD50 rat acute oral toxicity data. Journal of Cheminformatics, 2019, 11, 58.	2.8	71
23	Integrating in silico models for the prediction of mutagenicity (Ames test) of botanical ingredients of cosmetics. Computational Toxicology, 2019, 12, 100108.	1.8	10
24	QSAR Development for Plasma Protein Binding: Influence of the Ionization State. Pharmaceutical Research, 2019, 36, 28.	1.7	11
25	Integrating QSAR, Read-Across, and Screening Tools: The VEGAHUB Platform as an Example. Challenges and Advances in Computational Chemistry and Physics, 2019, , 365-381.	0.6	11
26	Development, validation and integration of in silico models to identify androgen active chemicals. Chemosphere, 2019, 220, 204-215.	4.2	23
27	Impact of REACH legislation on the production and importation of CMR (carcinogen, mutagen and) Tj ETQq1 1 0.784314 rgBT /Overlock Pharmacology, 2019, 101, 166-171.	1.3	1
28	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.	2.5	61
29	Prediction of Biochemical Endpoints by the CORAL Software: Prejudices, Paradoxes, and Results. Methods in Molecular Biology, 2018, 1800, 573-583.	0.4	6
30	A large comparison of integrated SAR/QSAR models of the Ames test for mutagenicity[$]. SAR and QSAR in Environmental Research, 2018, 29, 591-611.	1.0	21
31	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	2.8	264
32	Integrating in silico models to enhance predictivity for developmental toxicity. Toxicology, 2016, 370, 127-137.	2.0	39
33	Integrated in silico strategy for PBT assessment and prioritization under REACH. Environmental Research, 2016, 151, 478-492.	3.7	32
34	In Silico Model for Developmental Toxicity: How to Use QSAR Models and Interpret Their Results. Methods in Molecular Biology, 2016, 1425, 139-161.	0.4	7
35	In silicotools 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.	1.0	9
36	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.	2.9	24

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37	Comparison ofin silicotools for evaluating rat oral acute toxicity. SAR and QSAR in Environmental Research, 2015, 26, 1-27.	1.0	87
38	Evaluation and comparison of benchmark QSAR models to predict a relevant REACH endpoint: The bioconcentration factor (BCF). Environmental Research, 2015, 137, 398-409.	3.7	42
39	Integrating QSAR and read-across for environmental assessment. SAR and QSAR in Environmental Research, 2015, 26, 605-618.	1.0	17
40	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
41	Optimizing the aquatic toxicity assessment under REACH through an integrated testing strategy (ITS). Environmental Research, 2014, 135, 156-164.	3.7	11
42	Integrated testing strategy (ITS) for bioaccumulation assessment under REACH. Environment International, 2014, 69, 40-50.	4.8	14
43	A comparative survey of chemistry-driven in silico methods to identify hazardous substances under REACH. Regulatory Toxicology and Pharmacology, 2013, 66, 301-314.	1.3	42
44	In silico methods to predict drug toxicity. Current Opinion in Pharmacology, 2013, 13, 802-806.	1.7	72
45	Quantitative consensus of bioaccumulation models for integrated testing strategies. Environment International, 2012, 45, 51-58.	4.8	41
46	CORAL: the prediction of biodegradation of organic compounds with optimal SMILES-based descriptors. Open Chemistry, 2012, 10, 1042-1048.	1.0	7
47	Coral: QSAR models for acute toxicity in fathead minnow (Pimephales promelas). Journal of Computational Chemistry, 2012, 33, 1218-1223.	1.5	23
48	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.	1.3	16
49	CORAL: Building up the model for bioconcentration factor and defining itâ€™s applicability domain. European Journal of Medicinal Chemistry, 2011, 46, 1400-1403.	2.6	57
50	Comparison and Possible Use ofIn SilicoTools for Carcinogenicity Within REACH Legislation. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2011, 29, 300-323.	2.9	24
51	A new bioconcentration factor model based on SMILES and indices of presence of atoms. European Journal of Medicinal Chemistry, 2010, 45, 4399-4402.	2.6	29
52	Assessment and validation of the CAESAR predictive model for bioconcentration factor (BCF) in fish. Chemistry Central Journal, 2010, 4, S1.	2.6	54
53	New public QSAR model for carcinogenicity. Chemistry Central Journal, 2010, 4, S3.	2.6	105
54	Global QSAR models of skin sensitisers for regulatory purposes. Chemistry Central Journal, 2010, 4, S5.	2.6	51

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55	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, 711-729.	1.0	18
56	Computer-aided methodologies to predict endocrine-disrupting potency of chemicals. , 2009, , 306-321.		0
57	In silico-aided prediction of biological properties of chemicals: oestrogen receptor-mediated effects. Chemical Society Reviews, 2008, 37, 441-450.	18.7	33
58	A comparison of DEMETRA individual QSARs with an index for evaluation of uncertainty. Chemosphere, 2008, 71, 1845-1852.	4.2	4
59	A new hybrid system of QSAR models for predicting bioconcentration factors (BCF). Chemosphere, 2008, 73, 1701-1707.	4.2	92
60	Regulatory Perspectives in the Use and Validation of QSAR. A Case Study: DEMETRA Model forDaphniaToxicity. Environmental Science & Technology, 2008, 42, 491-496.	4.6	21
61	Binary classification models for endocrine disrupter effects mediated through the estrogen receptor. SAR and QSAR in Environmental Research, 2008, 19, 697-733.	1.0	43
62	Databases for pesticide ecotoxicity. , 2007, , 59-81.		2
63	Validation of the models. , 2007, , 185-199.		9
64	Results of DEMETRA models. , 2007, , 201-281.		6
65	Ecotoxicity prediction by adaptive fuzzy partitioning: comparing descriptors computed on 2D and 3D structures. SAR and QSAR in Environmental Research, 2006, 17, 225-251.	1.0	13
66	Variable Selection and Interpretation in Structureâ˜'Affinity Correlation Modeling of Estrogen Receptor Binders. Journal of Chemical Information and Modeling, 2005, 45, 1507-1519.	2.5	61
67	Identification of the Structural Requirements of the Receptor-Binding Affinity of Diphenolic Azoles to Estrogen Receptors Î± and Î² by Three-Dimensional Quantitative Structureâ˜'Activity Relationship and Structureâ˜'Activity Relationship Analysis. Journal of Medicinal Chemistry, 2005, 48, 7628-7636.	2.9	21
68	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, 641-652.	0.7	19
69	Classification of Potential Endocrine Disrupters on the Basis of Molecular Structure Using a Nonlinear Modeling Method.. ChemInform, 2004, 35, no.	0.1	0
70	Classification of Potential Endocrine Disrupters on the Basis of Molecular Structure Using a Nonlinear Modeling Methodâ€. Journal of Chemical Information and Computer Sciences, 2004, 44, 300-309.	2.8	29
71	Predicting logP of pesticides using different software. Chemosphere, 2003, 53, 1155-1164.	4.2	94
72	Factors Influencing Predictive Models for Toxicology. SAR and QSAR in Environmental Research, 2001, 12, 593-603.	1.0	32