Ester Papa

List of Publications by Year
in descending order

67 papers	4,047 citations	136950 32 h-index	114465 63 g-index
71 all docs	71 docs citations	71 times ranked	3332 citing authors

#	Article	IF	Citations
1	Classification-based QSARs for predicting dietary biomagnification in fish. SAR and QSAR in Environmental Research, 2022, 33, 259-271.	2.2	5
2	<scp>QSARINS</scp>â€Chem standalone version: A new platformâ€independent software to profile chemicals forÂphysicoâ€chemical properties, fate, and toxicity. Journal of Computational Chemistry, 2021, 42, 1452-1460.	3.3	16
3	New BODIPYs for photodynamic therapy (PDT): Synthesis and activity on human cancer cell lines. Bioorganic and Medicinal Chemistry, 2020, 28, 115737.	3.0	20
4	Are In Silico Approaches Applicable As a First Step for the Prediction of e-Liquid Toxicity in e-Cigarettes?. Chemical Research in Toxicology, 2020, 33, 2381-2389.	3.3	1
5	Application of chemometric methods and QSAR models to support pesticide risk assessment starting from ecotoxicological datasets. Water Research, 2020, 174, 115583.	11.3	26
6	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
7	Celebrating 40 Years of Career. Molecular Informatics, 2019, 38, e1980831.	2.5	0
8	Topological QSAR Modelling of Carboxamides Repellent Activity to Aedes Aegypti. Molecular Informatics, 2019, 38, e1900029.	2.5	1
9	High-throughput evaluation of organic contaminant removal efficiency in a wastewater treatment plant using direct injection UHPLC-Orbitrap-MS/MS. Environmental Sciences: Processes and Impacts, 2018, 20, 561-571.	3.5	23
10	Development of human biotransformation QSARs and application for PBT assessment refinement. Food and Chemical Toxicology, 2018, 112, 535-543.	3.6	27
11	QSAR modeling of cumulative environmental end-points for the prioritization of hazardous chemicals. Environmental Sciences: Processes and Impacts, 2018, 20, 38-47.	3.5	34
12	Quantitative Prediction of Rat Hepatotoxicity by Molecular Structure. International Journal of Quantitative Structure-Property Relationships, 2018, 3, 49-60.	0.5	3
13	QSAR models for predicting the toxicity of piperidine derivatives againstAedes aegypti. SAR and QSAR in Environmental Research, 2017, 28, 451-470.	2.2	16
14	In Silico Approaches for the Prediction of In Vivo Biotransformation Rates. Challenges and Advances in Computational Chemistry and Physics, 2017, , 425-451.	0.6	1
15	Computational approaches for the prediction of the selective uptake of magnetofluorescent nanoparticles into human cells. RSC Advances, 2016, 6, 68806-68818.	3.6	8
16	Investigation of the influence of protein corona composition on gold nanoparticle bioactivity using machine learning approaches. SAR and QSAR in Environmental Research, 2016, 27, 521-538.	2.2	44
17	Modeling ready biodegradability of fragrance materials. Environmental Toxicology and Chemistry, 2015, 34, 1224-1231.	4.3	15
18	Linear and non-linear modelling of the cytotoxicity of TiO₂ and ZnO nanoparticles by empirical descriptors. SAR and QSAR in Environmental Research, 2015, 26, 647-665.	2.2	31

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19	The QSPR-THESAURUS: The Online Platform of the CADASTER Project. ATLA Alternatives To Laboratory Animals, 2014, 42, 13-24.	1.0	10
20	Assessing predictive uncertainty in comparative toxicity potentials of triazoles. Environmental Toxicology and Chemistry, 2014, 33, 293-301.	4.3	5
21	Semivolatile PAH and n-alkane gas/particle partitioning using the dual model: up-to-date coefficients and comparison with experimental data. Environmental Science and Pollution Research, 2014, 21, 10163-10173.	5.3	19
22	Metabolic biotransformation half-lives in fish: QSAR modeling and consensus analysis. Science of the Total Environment, 2014, 470-471, 1040-1046.	8.0	74
23	UNDERSTANDING QUANTITATIVE STRUCTUREâ€"PROPERTY RELATIONSHIPS UNCERTAINTY IN ENVIRONMENTAL FATE MODELING. Environmental Toxicology and Chemistry, 2013, 32, 1069-1076.	4.3	11
24	QSARINS: A new software for the development, analysis, and validation of QSAR MLR models. Journal of Computational Chemistry, 2013, 34, 2121-2132.	3.3	516
25	Daphnia and fish toxicity of (benzo)triazoles: Validated QSAR models, and interspecies quantitative activityâ€"activity modelling. Journal of Hazardous Materials, 2013, 258-259, 50-60.	12.4	95
26	QSAR prediction of the competitive interaction of emerging halogenated pollutants with human transthyretin^{Â£}. SAR and QSAR in Environmental Research, 2013, 24, 333-349.	2.2	21
27	Experimental Assessment of the Environmental Fate and Effects of Triazoles and Benzotriazole. ATLA Alternatives To Laboratory Animals, 2013, 41, 65-75.	1.0	32
28	Evaluation of CADASTER QSAR Models for the Aquatic Toxicity of (Benzo)triazoles and Prioritisation by Consensus Prediction. ATLA Alternatives To Laboratory Animals, 2013, 41, 49-64.	1.0	18
29	QSAR classification models for the screening of the endocrine-disrupting activity of perfluorinated compounds. SAR and QSAR in Environmental Research, 2012, 23, 207-220.	2.2	25
30	QSAR Modeling is not â€œPush a Button and Find a Correlationâ€• A Case Study of Toxicity of (Benzoâ€)triazoles on Algae. Molecular Informatics, 2012, 31, 817-835.	2.5	193
31	CADASTER QSPR Models for Predictions of Melting and Boiling Points of Perfluorinated Chemicals. Molecular Informatics, 2011, 30, 189-204.	2.5	32
32	On the Use of Local and Global QSPRs for the Prediction of Physicoâ€chemical Properties of Polybrominated Diphenyl Ethers. Molecular Informatics, 2011, 30, 232-240.	2.5	14
33	QSAR classification models for the prediction of endocrine disrupting activity of brominated flame retardants. Journal of Hazardous Materials, 2011, 190, 106-112.	12.4	53
34	Antiproliferative Pt(IV) complexes: synthesis, biological activity, and quantitative structureâ€"activity relationship modeling. Journal of Biological Inorganic Chemistry, 2010, 15, 1157-1169.	2.6	123
35	QSAR Modeling and Prediction of the Endocrine-Disrupting Potencies of Brominated Flame Retardants. Chemical Research in Toxicology, 2010, 23, 946-954.	3.3	41
36	QSPR as a support for the EU REACH regulation and rational design of environmentally safer chemicals: PBT identification from molecular structure. Green Chemistry, 2010, 12, 836.	9.0	65

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37	Development, Validation and Inspection of the Applicability Domain of QSPR Models for Physicochemical Properties of Polybrominated Diphenyl Ethers. QSAR and Combinatorial Science, 2009, 28, 790-796.	1.4	84
38	Quantitative structureâ€“activity relationship modelling of oral acute toxicity and cytotoxic activity of fragrance materials in rodents. SAR and QSAR in Environmental Research, 2009, 20, 767-779.	2.2	14
39	Screening of persistent organic pollutants by QSPR classification models: A comparative study. Journal of Molecular Graphics and Modelling, 2008, 27, 59-65.	2.4	23
40	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	5.4	258
41	Evaluation and QSAR modeling on multiple endpoints of estrogen activity based on different bioassays. Chemosphere, 2008, 70, 1889-1897.	8.2	34
42	Critical Assessment of QSAR Models of Environmental Toxicity against Tetrahymena pyriformis: Focusing on Applicability Domain and Overfitting by Variable Selection. Journal of Chemical Information and Modeling, 2008, 48, 1733-1746.	5.4	350
43	Externally validated QSPR modelling of VOC tropospheric oxidation by NO₃ radicals. SAR and QSAR in Environmental Research, 2008, 19, 655-668.	2.2	23
44	Prediction of PAH mutagenicity in human cells by QSAR classification. SAR and QSAR in Environmental Research, 2008, 19, 115-127.	2.2	32
45	Approaches for externally validated QSAR modelling of Nitrated Polycyclic Aromatic Hydrocarbon mutagenicity. SAR and QSAR in Environmental Research, 2007, 18, 169-178.	2.2	45
46	Quantitative structureâ€“activity relationship modeling of polycyclic aromatic hydrocarbon mutagenicity by classification methods based on holistic theoretical molecular descriptors. Ecotoxicology and Environmental Safety, 2007, 66, 353-361.	6.0	16
47	Linear QSAR regression models for the prediction of bioconcentration factors by physicochemical properties and structural theoretical molecular descriptors. Chemosphere, 2007, 67, 351-358.	8.2	74
48	Multivariate Chemical Mapping of Antibiotics and Identification of Structurally Representative Substances. Environmental Science & Technology, 2007, 41, 1653-1661.	10.0	9
49	Screening and Ranking of POPs for Global Half-Life:Â QSAR Approaches for Prioritization Based on Molecular Structure. Environmental Science & Technology, 2007, 41, 2833-2839.	10.0	68
50	Statistical external validation and consensus modeling: A QSPR case study for Koc prediction. Journal of Molecular Graphics and Modelling, 2007, 25, 755-766.	2.4	221
51	In silico screening of estrogen-like chemicals based on different nonlinear classification models. Journal of Molecular Graphics and Modelling, 2007, 26, 135-144.	2.4	38
52	QSAR Prediction of Estrogen Activity for a Large Set of Diverse Chemicals under the Guidance of OECD Principles. Chemical Research in Toxicology, 2006, 19, 1540-1548.	3.3	119
53	Comparison between 5,10,15,20-Tetraaryl- and 5,15-Diarylporphyrins as Photosensitizers:Â Synthesis, Photodynamic Activity, and Quantitative Structureâ˜'Activity Relationship Modeling. Journal of Medicinal Chemistry, 2006, 49, 3293-3304.	6.4	61
54	Accumulation of Persistent Organic Pollutants in Canopies of Different Forest Types:Â Role of Species Composition and Altitudinal-Temperature Gradient. Environmental Science & Technology, 2006, 40, 6580-6586.	10.0	33

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55	Analysis of Mosses and Soils for Quantifying Heavy Metal Concentrations in Sicily: A Multivariate and Spatial Analytical Approach. Environmental Science and Pollution Research, 2006, 13, 28-36.	5.3	29
56	Ranking of Phenols for Abiotic Oxidation in Aqueous Environment: a QSPR Approach. Annali Di Chimica, 2005, 95, 199-209.	0.6	3
57	An Update of the BCF QSAR Model Based on Theoretical Molecular Descriptors. QSAR and Combinatorial Science, 2005, 24, 953-960.	1.4	55
58	Statistically Validated QSARs, Based on Theoretical Descriptors, for Modeling Aquatic Toxicity of Organic Chemicals in Pimephales promelas (Fathead Minnow). Journal of Chemical Information and Modeling, 2005, 45, 1256-1266.	5.4	169
59	Ranking of aquatic toxicity of esters modelled by QSAR. Chemosphere, 2005, 58, 559-570.	8.2	47
60	Ranking and classification of non-ionic organic pesticides for environmental distribution: a qsar approach. International Journal of Environmental Analytical Chemistry, 2004, 84, 65-74.	3.3	11
61	A tool for the assessment of VOC degradability by tropospheric oxidants starting from chemical structure. Atmospheric Environment, 2004, 38, 6167-6175.	4.1	54
62	Validated QSAR Prediction of OH Tropospheric Degradation of VOCs:â€‰ Splitting into Trainingâ^'Test Sets and Consensus Modeling. Journal of Chemical Information and Computer Sciences, 2004, 44, 1794-1802.	2.8	206
63	Screening the leaching tendency of pesticides applied in the Amu Darya Basin (Uzbekistan). Water Research, 2004, 38, 3485-3494.	11.3	44
64	Predicting the NO3 radical tropospheric degradability of organic pollutants by theoretical molecular descriptors. Atmospheric Environment, 2003, 37, 3115-3124.	4.1	39
65	QSAR Prediction of Ozone Tropospheric Degradation. QSAR and Combinatorial Science, 2003, 22, 364-373.	1.4	43
66	QSAR Modeling of Bioconcentration Factor by theoretical molecular descriptors. QSAR and Combinatorial Science, 2003, 22, 374-385.	1.4	85
67	Ranking of volatile organic compounds for tropospheric degradability by oxidants: A QSPR approach. SAR and QSAR in Environmental Research, 2002, 13, 743-753.	2.2	20