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	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
2	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
3	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	5.4	258
4	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
5	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
6	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
7	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
8	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
9	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
10	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
11	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
12	QSAR Modeling of Bioconcentration Factor by theoretical molecular descriptors. QSAR and Combinatorial Science, 2003, 22, 374-385.	1.4	85
13	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
14	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
15	Metabolic biotransformation half-lives in fish: QSAR modeling and consensus analysis. Science of the Total Environment, 2014, 470-471, 1040-1046.	8.0	74
16	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
17	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
18	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

#	Article	IF	Citations
19	An Update of the BCF QSAR Model Based on Theoretical Molecular Descriptors. QSAR and Combinatorial Science, 2005, 24, 953-960.	1.4	55
20	A tool for the assessment of VOC degradability by tropospheric oxidants starting from chemical structure. Atmospheric Environment, 2004, 38, 6167-6175.	4.1	54
21	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
22	Ranking of aquatic toxicity of esters modelled by QSAR. Chemosphere, 2005, 58, 559-570.	8.2	47
23	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
24	Screening the leaching tendency of pesticides applied in the Amu Darya Basin (Uzbekistan). Water Research, 2004, 38, 3485-3494.	11.3	44
25	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
26	QSAR Prediction of Ozone Tropospheric Degradation. QSAR and Combinatorial Science, 2003, 22, 364-373.	1.4	43
27	QSAR Modeling and Prediction of the Endocrine-Disrupting Potencies of Brominated Flame Retardants. Chemical Research in Toxicology, 2010, 23, 946-954.	3.3	41
28	Predicting the NO3 radical tropospheric degradability of organic pollutants by theoretical molecular descriptors. Atmospheric Environment, 2003, 37, 3115-3124.	4.1	39
29	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
30	Evaluation and QSAR modeling on multiple endpoints of estrogen activity based on different bioassays. Chemosphere, 2008, 70, 1889-1897.	8.2	34
31	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
32	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
33	Prediction of PAH mutagenicity in human cells by QSAR classification. SAR and QSAR in Environmental Research, 2008, 19, 115-127.	2.2	32
34	CADASTER QSPR Models for Predictions of Melting and Boiling Points of Perfluorinated Chemicals. Molecular Informatics, 2011, 30, 189-204.	2.5	32
35	Experimental Assessment of the Environmental Fate and Effects of Triazoles and Benzotriazole. ATLA Alternatives To Laboratory Animals, 2013, 41, 65-75.	1.0	32
36	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

#	Article	IF	Citations
37	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
38	Development of human biotransformation QSARs and application for PBT assessment refinement. Food and Chemical Toxicology, 2018, 112, 535-543.	3.6	27
39	Application of chemometric methods and QSAR models to support pesticide risk assessment starting from ecotoxicological datasets. Water Research, 2020, 174, 115583.	11.3	26
40	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
41	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
42	Externally validated QSPR modelling of VOC tropospheric oxidation by NO₃ radicals. SAR and QSAR in Environmental Research, 2008, 19, 655-668.	2.2	23
43	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
44	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
45	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
46	New BODIPYs for photodynamic therapy (PDT): Synthesis and activity on human cancer cell lines. Bioorganic and Medicinal Chemistry, 2020, 28, 115737.	3.0	20
47	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
48	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
49	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
50	QSAR models for predicting the toxicity of piperidine derivatives againstAedes aegypti. SAR and QSAR in Environmental Research, 2017, 28, 451-470.	2.2	16
51	<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
52	Modeling ready biodegradability of fragrance materials. Environmental Toxicology and Chemistry, 2015, 34, 1224-1231.	4.3	15
53	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
54	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

#	Article	IF	Citations
55	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
56	UNDERSTANDING QUANTITATIVE STRUCTUREâ€“PROPERTY RELATIONSHIPS UNCERTAINTY IN ENVIRONMENTAL FATE MODELING. Environmental Toxicology and Chemistry, 2013, 32, 1069-1076.	4.3	11
57	The QSPR-THESAURUS: The Online Platform of the CADASTER Project. ATLA Alternatives To Laboratory Animals, 2014, 42, 13-24.	1.0	10
58	Multivariate Chemical Mapping of Antibiotics and Identification of Structurally Representative Substances. Environmental Science & Technology, 2007, 41, 1653-1661.	10.0	9
59	Computational approaches for the prediction of the selective uptake of magnetofluorescent nanoparticles into human cells. RSC Advances, 2016, 6, 68806-68818.	3.6	8
60	Assessing predictive uncertainty in comparative toxicity potentials of triazoles. Environmental Toxicology and Chemistry, 2014, 33, 293-301.	4.3	5
61	Classification-based QSARs for predicting dietary biomagnification in fish. SAR and QSAR in Environmental Research, 2022, 33, 259-271.	2.2	5
62	Ranking of Phenols for Abiotic Oxidation in Aqueous Environment: a QSPR Approach. Annali Di Chimica, 2005, 95, 199-209.	0.6	3
63	Quantitative Prediction of Rat Hepatotoxicity by Molecular Structure. International Journal of Quantitative Structure-Property Relationships, 2018, 3, 49-60.	0.5	3
64	Topological QSAR Modelling of Carboxamides Repellent Activity to Aedes Aegypti. Molecular Informatics, 2019, 38, e1900029.	2.5	1
65	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
66	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
67	Celebrating 40 Years of Career. Molecular Informatics, 2019, 38, e1980831.	2.5	0