Paola Gramatica

List of Publications by Year
in descending order

134	15,648	36303 51	16650 123
papers	citations	h-index	g-index

138	138	138	9652
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Importance of Being Earnest: Validation is the Absolute Essential for Successful Application and Interpretation of QSPR Models. QSAR and Combinatorial Science, 2003, 22, 69-77.	1.4	1,698
2	Principles of QSAR models validation: internal and external. QSAR and Combinatorial Science, 2007, 26, 694-701.	1.4	1,644
3	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	6.4	1,401
4	Methods for reliability and uncertainty assessment and for applicability evaluations of classification- and regression-based QSARs.. Environmental Health Perspectives, 2003, 111, 1361-1375.	6.0	1,108
5	Real External Predictivity of QSAR Models: How To Evaluate It? Comparison of Different Validation Criteria and Proposal of Using the Concordance Correlation Coefficient. Journal of Chemical Information and Modeling, 2011, 51, 2320-2335.	5.4	589
6	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
7	Real External Predictivity of QSAR Models. Part 2. New Intercomparable Thresholds for Different Validation Criteria and the Need for Scatter Plot Inspection. Journal of Chemical Information and Modeling, 2012, 52, 2044-2058.	5.4	408
8	Joint algal toxicity of 16 dissimilarly acting chemicals is predictable by the concept of independent action. Aquatic Toxicology, 2003, 63, 43-63.	4.0	379
9	Predicting the joint algal toxicity of multi-component s-triazine mixtures at low-effect concentrations of individual toxicants. Aquatic Toxicology, 2001, 56, 13-32.	4.0	357
10	A Historical Excursus on the Statistical Validation Parameters for QSAR Models: A Clarification Concerning Metrics and Terminology. Journal of Chemical Information and Modeling, 2016, 56, 1127-1131.	5.4	308
11	Structure/Response Correlations and Similarity/Diversity Analysis by GETAWAY Descriptors. 2. Application of the Novel 3D Molecular Descriptors to QSAR/QSPR Studies. Journal of Chemical Information and Computer Sciences, 2002, 42, 693-705.	2.8	278
12	QSARINSâ€¢chem: Insubria datasets and new QSAR/QSPR models for environmental pollutants in QSARINS. Journal of Computational Chemistry, 2014, 35, 1036-1044.	3.3	271
13	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	5.4	258
14	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
15	Validated QSAR Prediction of OH Tropospheric Degradation of VOCs:â€‰ Splitting into Trainingâˆ’Test Sets and Consensus Modeling. Journal of Chemical Information and Computer Sciences, 2004, 44, 1794-1802.	2.8	206
16	Applicability Domains for Classification Problems: Benchmarking of Distance to Models for Ames Mutagenicity Set. Journal of Chemical Information and Modeling, 2010, 50, 2094-2111.	5.4	202
17	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
18	On the Development and Validation of QSAR Models. Methods in Molecular Biology, 2013, 930, 499-526.	0.9	173

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19	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
20	JOINT ALGAL TOXICITY OF PHENYLUREA HERBICIDES IS EQUALLY PREDICTABLE BY CONCENTRATION ADDITION AND INDEPENDENT ACTION. Environmental Toxicology and Chemistry, 2004, 23, 258.	4.3	149
21	SD-modelling and Prediction by WHIM Descriptors. Part 5. Theory Development and Chemical Meaning of WHIM Descriptors. QSAR and Combinatorial Science, 1997, 16, 113-119.	1.2	141
22	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
23	Mixture toxicity of priority pollutants at no observed effect concentrations (NOECs). Ecotoxicology, 2002, 11, 299-310.	2.4	120
24	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
25	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
26	Principles of QSAR Modeling. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 61-97.	0.5	115
27	Prediction of Aqueous Solubility, Vapor Pressure and Critical Micelle Concentration for Aquatic Partitioning of Perfluorinated Chemicals. Environmental Science & Technology, 2011, 45, 8120-8128.	10.0	112
28	The BEAM-project: prediction and assessment of mixture toxicities in the aquatic environment. Continental Shelf Research, 2003, 23, 1757-1769.	1.8	111
29	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
30	Hazard of pharmaceuticals for aquatic environment: Prioritization by structural approaches and prediction of ecotoxicity. Environment International, 2016, 95, 131-143.	10.0	95
31	QSAR Modeling of Bioconcentration Factor by theoretical molecular descriptors. QSAR and Combinatorial Science, 2003, 22, 374-385.	1.4	85
32	External Evaluation of QSAR Models, in Addition to Crossâ€Validation: Verification of Predictive Capability on Totally New Chemicals. Molecular Informatics, 2014, 33, 311-314.	2.5	85
33	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
34	Water quality objectives for mixtures of toxic chemicals: problems and perspectives. Ecotoxicology and Environmental Safety, 2003, 54, 139-150.	6.0	83
35	Stereospecific reduction of geraniol to (R)-(+)-citronellol bySaccharomyces cerevisiae. Experientia, 1982, 38, 775-776.	1.2	78
36	PBT assessment and prioritization of contaminants of emerging concern: Pharmaceuticals. Environmental Research, 2016, 147, 297-306.	7.5	75

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37	QSAR study of selective ligands for the thyroid hormone receptor Î². Bioorganic and Medicinal Chemistry, 2007, 15, 5251-5261.	3.0	74
38	Metabolic biotransformation half-lives in fish: QSAR modeling and consensus analysis. Science of the Total Environment, 2014, 470-471, 1040-1046.	8.0	74
39	Aquatic ecotoxicity of personal care products: QSAR models and ranking for prioritization and safer alternativesâ€™ design. Green Chemistry, 2016, 18, 4393-4406.	9.0	74
40	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
41	QSAR study on the tropospheric degradation of organic compounds. Chemosphere, 1999, 38, 1371-1378.	8.2	67
42	QSAR model reproducibility and applicability: A case study of rate constants of hydroxyl radical reaction models applied to polybrominated diphenyl ethers and (benzoâ€)triazoles. Journal of Computational Chemistry, 2011, 32, 2386-2396.	3.3	66
43	3D-modelling and Prediction by WHIM Descriptors. Part 6. Application of WHIM Descriptors in QSAR Studies. QSAR and Combinatorial Science, 1997, 16, 120-125.	1.2	65
44	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
45	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
46	Chiral synthetic intermediates via asymmetric hydrogenation of .alpha.-methyl-.alpha.,.beta.-unsaturated aldehydes by bakers' yeast. Journal of Organic Chemistry, 1985, 50, 4625-4628.	3.2	59
47	Screening of pesticides for environmental partitioning tendency. Chemosphere, 2002, 47, 947-956.	8.2	59
48	An Update of the BCF QSAR Model Based on Theoretical Molecular Descriptors. QSAR and Combinatorial Science, 2005, 24, 953-960.	1.4	55
49	Are some â€œsafer alternativesâ€•hazardous as PBTs? The case study of new flame retardants. Journal of Hazardous Materials, 2016, 306, 237-246.	12.4	54
50	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
51	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, 265-284.	2.2	50
52	Aloeresin c, a bitter c,o-diglucoside from cape aloe. Phytochemistry, 1985, 24, 1571-1573.	2.9	48
53	Classification of organic solvents and modelling of their physico-chemical properties by chemometric methods using different sets of molecular descriptors. TrAC - Trends in Analytical Chemistry, 1999, 18, 461-471.	11.4	48
54	PBT assessment and prioritization by PBT Index and consensus modeling: Comparison of screening results from structural models. Environment International, 2015, 77, 25-34.	10.0	48

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55	Ranking of aquatic toxicity of esters modelled by QSAR. Chemosphere, 2005, 58, 559-570.	8.2	47
56	QSAR study of malonylâ€CoA decarboxylase inhibitors using GAâ€MLR and a new strategy of consensus modeling. Journal of Computational Chemistry, 2008, 29, 2636-2647.	3.3	46
57	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
58	Screening the leaching tendency of pesticides applied in the Amu Darya Basin (Uzbekistan). Water Research, 2004, 38, 3485-3494.	11.3	44
59	A C-glucosylated 5-methylchromone from Kenya aloe. Phytochemistry, 1986, 25, 2219-2222.	2.9	43
60	QSAR Prediction of Ozone Tropospheric Degradation. QSAR and Combinatorial Science, 2003, 22, 364-373.	1.4	43
61	QSAR and Chemometric Approaches for Setting Water Quality Objectives for Dangerous Chemicals. Ecotoxicology and Environmental Safety, 2001, 49, 206-220.	6.0	42
62	Identification of potential PBT behavior of personal care products by structural approaches. Sustainable Chemistry and Pharmacy, 2015, 1, 19-27.	3.3	42
63	Stereoselective total synthesis of natural phytol double bond reductions by baker's yeast. Tetrahedron, 1987, 43, 4481-4486.	1.9	41
64	QSAR Modeling and Prediction of the Endocrine-Disrupting Potencies of Brominated Flame Retardants. Chemical Research in Toxicology, 2010, 23, 946-954.	3.3	41
65	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
66	The importance of molecular structures, endpointsâ€™ values, and predictivity parameters in QSAR research: QSAR analysis of a series of estrogen receptor binders. Molecular Diversity, 2010, 14, 687-696.	3.9	38
67	Classification and Virtual Screening of Androgen Receptor Antagonists. Journal of Chemical Information and Modeling, 2010, 50, 861-874.	5.4	38
68	Reaction of nitroolefins with raney nickel and sodium hypophosphite. A mild method for converting nitroolefins into ketones (or aldehydes).. Tetrahedron Letters, 1983, 24, 417-418.	1.4	36
69	Per- and Polyfluoro Toxicity (LC₅₀ Inhalation) Study in Rat and Mouse Using QSAR Modeling. Chemical Research in Toxicology, 2010, 23, 528-539.	3.3	35
70	Evaluation and QSAR modeling on multiple endpoints of estrogen activity based on different bioassays. Chemosphere, 2008, 70, 1889-1897.	8.2	34
71	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
72	Steric Control of Conductivity in Highly Conjugated Polythiophenes. Chemistry of Materials, 2001, 13, 1665-1673.	6.7	33

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73	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
74	Integrated QSPR models to predict the soil sorption coefficient for a large diverse set of compounds by using different modeling methods. Atmospheric Environment, 2014, 88, 212-218.	4.1	33
75	Prediction of PAH mutagenicity in human cells by QSAR classification. SAR and QSAR in Environmental Research, 2008, 19, 115-127.	2.2	32
76	CADASTER QSPR Models for Predictions of Melting and Boiling Points of Perfluorinated Chemicals. Molecular Informatics, 2011, 30, 189-204.	2.5	32
77	Modelling physico-chemical properties of (benzo)triazoles, and screening for environmental partitioning. Water Research, 2011, 45, 1463-1471.	11.3	31
78	Singlet oxygen reactions in aqueous solution. Physical and chemical quenching rate constants of crocin and related carotenoids. Tetrahedron Letters, 1987, 28, 4221-4224.	1.4	30
79	Prediction of aromatic amines mutagenicity from theoretical molecular descriptors. SAR and QSAR in Environmental Research, 2003, 14, 237-250.	2.2	30
80	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
81	QSAR classification of estrogen receptor binders and pre-screening of potential pleiotropic EDCs. SAR and QSAR in Environmental Research, 2010, 21, 657-669.	2.2	29
82	Oral LD50 toxicity modeling and prediction of per- and polyfluorinated chemicals on rat and mouse. Molecular Diversity, 2011, 15, 467-476.	3.9	29
83	New 3D Molecular Descriptors: The WHIM theory and QSAR Applications. , 2002, , 355-380.		28
84	Development of human biotransformation QSARs and application for PBT assessment refinement. Food and Chemical Toxicology, 2018, 112, 535-543.	3.6	27
85	Biosynthesis of phenylpropanoid compounds. Part I. Biosynthesis of eugenol in Ocimum basilicum L. Journal of the Chemical Society Perkin Transactions 1, 1974, , 1727.	0.9	26
86	Decarboxylation of cinnamic acids by Saccharomyces cerevisiae. Bioorganic Chemistry, 1981, 10, 14-21.	4.1	25
87	Correlations and complementarities in data and methods through Principal Components Analysis (PCA) applied to the results of the SPIn-Eco Project. Journal of Environmental Management, 2008, 86, 419-426.	7.8	25
88	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
89	Structural requirements of 3-carboxyl-4(1H)-quinolones as potential antimalarials from 2D and 3D QSAR analysis. Journal of Molecular Graphics and Modelling, 2013, 44, 266-277.	2.4	25
90	Synthesis, photodynamic activity, and quantitative structure-activity relationship modelling of a series of BODIPYs. Journal of Photochemistry and Photobiology B: Biology, 2017, 167, 269-281.	3.8	25

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91	BAKERâ€™S YEAST HYDROGENATION OF CARBONYL ACTIVATED DOUBLE BONDS. ENANTIOSELECTIVE SYNTHESIS OF THE (S)-FORM OF THE DIHYDROTERPENEDIOL SECRETED BYDANAUS CHRYSIPPUSAND OF A PHEROMONE OFCALLOSOBRUCHUS CHINENSISL.. Chemistry Letters, 1985, 14, 1395-1398.	1.3	24
92	Prediction of infinite-dilution activity coefficients of organic solutes in ionic liquids using temperature-dependent quantitative structureâ€“property relationship method. Chemical Engineering Journal, 2010, 163, 195-201.	12.7	24
93	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
94	Externally validated QSPR modelling of VOC tropospheric oxidation by NO₃ radicals. SAR and QSAR in Environmental Research, 2008, 19, 655-668.	2.2	23
95	Prediction of the adsorption capability onto activated carbon of a large data set of chemicals by local lazy regression method. Atmospheric Environment, 2010, 44, 2954-2960.	4.1	22
96	Tautomerism and multiple modelling enhance the efficacy of QSAR: antimalarial activity of phosphoramidate and phosphorothioamidate analogues of amiprophos methyl. Medicinal Chemistry Research, 2014, 23, 4825-4835.	2.4	22
97	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
98	WHIM Descriptors of Shape. QSAR and Combinatorial Science, 2006, 25, 327-332.	1.4	20
99	A convenient synthesis of both the anomers of ethyl (2,3,4,6-tetra-O-benzyl-D-glucopyranosyl)acetate. Tetrahedron Letters, 1987, 28, 5047-5048.	1.4	19
100	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
101	Chemometric Methods and Theoretical Molecular Descriptors in Predictive QSAR Modeling of the Environmental Behavior of Organic Pollutants. Challenges and Advances in Computational Chemistry and Physics, 2010, , 327-366.	0.6	17
102	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
103	<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
104	Modeling ready biodegradability of fragrance materials. Environmental Toxicology and Chemistry, 2015, 34, 1224-1231.	4.3	15
105	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
106	The Applications of Machine Learning Algorithms in the Modeling of Estrogen-Like Chemicals. Combinatorial Chemistry and High Throughput Screening, 2009, 12, 490-496.	1.1	14
107	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
108	Reduction of cinnamyl alcohols and cinnamaldehydes by Saccharomyces cerevisiae. Bioorganic Chemistry, 1981, 10, 22-28.	4.1	13

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109	In Memory of Professor Davide Calamari. Environmental Science and Pollution Research, 2006, 13, 1-1.	5.3	13
110	Stereochemistry of the decarboxylation of phenolic cinnamic acids by Saccharomyces cerevisiae. Journal of the Chemical Society Chemical Communications, 1975, , 442.	2.0	12
111	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
112	Are Mechanistic and Statistical QSAR Approaches Really Different? MLR Studies on 158 Cycloalkylâ€Pyranones. Molecular Informatics, 2010, 29, 511-522.	2.5	11
113	Biosynthesis of anethole in L.. Tetrahedron Letters, 1974, 15, 1567-1568.	1.4	10
114	QSAR modelling of water quality indices of alkylphenol pollutants. SAR and QSAR in Environmental Research, 2007, 18, 729-743.	2.2	10
115	The QSPR-THESAURUS: The Online Platform of the CADASTER Project. ATLA Alternatives To Laboratory Animals, 2014, 42, 13-24.	1.0	10
116	A Combined Quantitative Structure-Activity Relationship Research of Quinolinone Derivatives as Androgen Receptor Antagonists. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 834-845.	1.1	10
117	Multivariate Chemical Mapping of Antibiotics and Identification of Structurally Representative Substances. Environmental Science & Technology, 2007, 41, 1653-1661.	10.0	9
118	New QSAR Modelling Approach Based on Ranking Models by Genetic Algorithms - Variable Subset Selection (GA-VSS). , 2006, , 181-217.		8
119	Preparation of cinnamic acids labelled with deuterium or tritium at the Î±-position. Journal of the Chemical Society Chemical Communications, 1973, , 563-564.	2.0	7
120	Toward an in Vitro Test for the Diagnosis of Allergy to Penicillins. Synthesis, Characterization, and Use of Î²-Lactam and Î²-Lactam Metabolite Poly-l-lysines Which Recognize Human IgE Antibodies. Bioconjugate Chemistry, 1999, 10, 332-337.	3.6	7
121	Combined Ligand/Structure-Based Virtual Screening and Molecular Dynamics Simulations of Steroidal Androgen Receptor Antagonists. BioMed Research International, 2017, 2017, 1-18.	1.9	7
122	Synthesis of (2S, 5R) - [5-2H] Proline. Journal of Labelled Compounds and Radiopharmaceuticals, 1981, 18, 955-962.	1.0	6
123	Structureâ€Activity Relationship Analysis of the Thermal Stabilities of Nitroaromatic Compounds Following Different Decomposition Mechanisms. Molecular Informatics, 2013, 32, 193-202.	2.5	5
124	Ligand Efficiency Outperforms <scp>pIC</scp>₅₀ on Both 2D <scp>MLR</scp> and 3D Co<scp>MFA</scp> Models: A Case Study on <scp>AR</scp> Antagonists. Chemical Biology and Drug Design, 2015, 86, 1501-1517.	3.2	5
125	Ranking of Phenols for Abiotic Oxidation in Aqueous Environment: a QSPR Approach. Annali Di Chimica, 2005, 95, 199-209.	0.6	3
126	A new strategy to improve the predictive ability of the local lazy regression and its application to the QSAR study of melaninâ€concentrating hormone receptor 1 antagonists. Journal of Computational Chemistry, 2010, 31, 973-985.	3.3	3

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127	Quantitative Prediction of Rat Hepatotoxicity by Molecular Structure. International Journal of Quantitative Structure-Property Relationships, 2018, 3, 49-60.	0.5	3
128	Chapter 17. Modelling Chemicals in the Environment. RSC Drug Discovery Series, 0, , 458-478.	0.3	2
129	Reply to the comment of S. Rayne on â€œQSAR model reproducibility and applicability: A case study of rate constants of hydroxyl radical reaction models applied to polybrominated diphenyl ethers and (benzoâ€)triazolesâ€. Journal of Computational Chemistry, 2013, 34, 1796-1796.	3.3	2
130	Prioritization of Chemicals Based on Chemoinformatic Analysis. , 2016, , 1-33.		2
131	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
132	Biosynthesis of caffeic acid in Ocimum basilicum L.. Journal of the Chemical Society Chemical Communications, 1979, , 1073b.	2.0	0
133	Quantitative structureâ€“activity relationship analysis of a novel series of chemicals antagonizing WT and MT AR. Chemometrics and Intelligent Laboratory Systems, 2011, 107, 283-289.	3.5	0
134	Prioritization of Chemicals Based on Chemoinformatic Analysis. , 2017, , 2231-2263.		0