

# Paola Gramatica

## List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	The Importance of Being Earnest: Validation is the Absolute Essential for Successful Application and Interpretation of QSPR Models. <i>QSAR and Combinatorial Science</i> , 2003, 22, 69-77.	1.4	1,698
2	Principles of QSAR models validation: internal and external. <i>QSAR and Combinatorial Science</i> , 2007, 26, 694-701.	1.4	1,644
3	QSAR Modeling: Where Have You Been? Where Are You Going To?. <i>Journal of Medicinal Chemistry</i> , 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.. <i>Environmental Health Perspectives</i> , 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. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2320-2335.	5.4	589
6	QSARINS: A new software for the development, analysis, and validation of QSAR MLR models. <i>Journal of Computational Chemistry</i> , 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. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 2044-2058.	5.4	408
8	Joint algal toxicity of 16 dissimilarly acting chemicals is predictable by the concept of independent action. <i>Aquatic Toxicology</i> , 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. <i>Aquatic Toxicology</i> , 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. <i>Journal of Chemical Information and Modeling</i> , 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. <i>Journal of Chemical Information and Computer Sciences</i> , 2002, 42, 693-705.	2.8	278
12	QSARINS@Chem: Insubria datasets and new QSAR/QSPR models for environmental pollutants in QSARINS. <i>Journal of Computational Chemistry</i> , 2014, 35, 1036-1044.	3.3	271
13	Combinatorial QSAR Modeling of Chemical Toxicants Tested against <i>Tetrahymena pyriformis</i> . <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 766-784.	5.4	258
14	Statistical external validation and consensus modeling: A QSPR case study for Koc prediction. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 25, 755-766.	2.4	221
15	Validated QSAR Prediction of OH Tropospheric Degradation of VOCs: Splitting into Training and Test Sets and Consensus Modeling. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 1794-1802.	2.8	206
16	Applicability Domains for Classification Problems: Benchmarking of Distance to Models for Ames Mutagenicity Set. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 2094-2111.	5.4	202
17	QSAR Modeling is not "Push a Button and Find a Correlation": A Case Study of Toxicity of (Benzo)triazoles on Algae. <i>Molecular Informatics</i> , 2012, 31, 817-835.	2.5	193
18	On the Development and Validation of QSAR Models. <i>Methods in Molecular Biology</i> , 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). <i>Journal of Chemical Information and Modeling</i> , 2005, 45, 1256-1266.	5.4	169
20	JOINT ALGAL TOXICITY OF PHENYLUREA HERBICIDES IS EQUALLY PREDICTABLE BY CONCENTRATION ADDITION AND INDEPENDENT ACTION. <i>Environmental Toxicology and Chemistry</i> , 2004, 23, 258.	4.3	149
21	SD-modelling and Prediction by WHIM Descriptors. Part 5. Theory Development and Chemical Meaning of WHIM Descriptors. <i>QSAR and Combinatorial Science</i> , 1997, 16, 113-119.	1.2	141
22	Antiproliferative Pt(IV) complexes: synthesis, biological activity, and quantitative structure-activity relationship modeling. <i>Journal of Biological Inorganic Chemistry</i> , 2010, 15, 1157-1169.	2.6	123
23	Mixture toxicity of priority pollutants at no observed effect concentrations (NOECs). <i>Ecotoxicology</i> , 2002, 11, 299-310.	2.4	120
24	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. <i>Environmental Health Perspectives</i> , 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. <i>Chemical Research in Toxicology</i> , 2006, 19, 1540-1548.	3.3	119
26	Principles of QSAR Modeling. <i>International Journal of Quantitative Structure-Property Relationships</i> , 2020, 5, 61-97.	0.5	115
27	Prediction of Aqueous Solubility, Vapor Pressure and Critical Micelle Concentration for Aquatic Partitioning of Perfluorinated Chemicals. <i>Environmental Science &amp; Technology</i> , 2011, 45, 8120-8128.	10.0	112
28	The BEAM-project: prediction and assessment of mixture toxicities in the aquatic environment. <i>Continental Shelf Research</i> , 2003, 23, 1757-1769.	1.8	111
29	Daphnia and fish toxicity of (benzo)triazoles: Validated QSAR models, and interspecies quantitative activity-activity modelling. <i>Journal of Hazardous Materials</i> , 2013, 258-259, 50-60.	12.4	95
30	Hazard of pharmaceuticals for aquatic environment: Prioritization by structural approaches and prediction of ecotoxicity. <i>Environment International</i> , 2016, 95, 131-143.	10.0	95
31	QSAR Modeling of Bioconcentration Factor by theoretical molecular descriptors. <i>QSAR and Combinatorial Science</i> , 2003, 22, 374-385.	1.4	85
32	External Evaluation of QSAR Models, in Addition to Cross-validation: Verification of Predictive Capability on Totally New Chemicals. <i>Molecular Informatics</i> , 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. <i>QSAR and Combinatorial Science</i> , 2009, 28, 790-796.	1.4	84
34	Water quality objectives for mixtures of toxic chemicals: problems and perspectives. <i>Ecotoxicology and Environmental Safety</i> , 2003, 54, 139-150.	6.0	83
35	Stereospecific reduction of geraniol to (R)-(+)-citronellol by <i>Saccharomyces cerevisiae</i> . <i>Experientia</i> , 1982, 38, 775-776.	1.2	78
36	PBT assessment and prioritization of contaminants of emerging concern: Pharmaceuticals. <i>Environmental Research</i> , 2016, 147, 297-306.	7.5	75

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37	QSAR study of selective ligands for the thyroid hormone receptor $\beta$ . <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 5251-5261.	3.0	74
38	Metabolic biotransformation half-lives in fish: QSAR modeling and consensus analysis. <i>Science of the Total Environment</i> , 2014, 470-471, 1040-1046.	8.0	74
39	Aquatic ecotoxicity of personal care products: QSAR models and ranking for prioritization and safer alternatives™ design. <i>Green Chemistry</i> , 2016, 18, 4393-4406.	9.0	74
40	Screening and Ranking of POPs for Global Half-Life: QSAR Approaches for Prioritization Based on Molecular Structure. <i>Environmental Science &amp; Technology</i> , 2007, 41, 2833-2839.	10.0	68
41	QSAR study on the tropospheric degradation of organic compounds. <i>Chemosphere</i> , 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 (benzo)triazoles. <i>Journal of Computational Chemistry</i> , 2011, 32, 2386-2396.	3.3	66
43	3D-modelling and Prediction by WHIM Descriptors. Part 6. Application of WHIM Descriptors in QSAR Studies. <i>QSAR and Combinatorial Science</i> , 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. <i>Green Chemistry</i> , 2010, 12, 836.	9.0	65
45	Comparison between 5,10,15,20-Tetraaryl- and 5,15-Diarylporphyrins as Photosensitizers: Synthesis, Photodynamic Activity, and Quantitative Structure-Activity Relationship Modeling. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 3293-3304.	6.4	61
46	Chiral synthetic intermediates via asymmetric hydrogenation of $\alpha$ -methyl- $\alpha,\beta$ -unsaturated aldehydes by bakers' yeast. <i>Journal of Organic Chemistry</i> , 1985, 50, 4625-4628.	3.2	59
47	Screening of pesticides for environmental partitioning tendency. <i>Chemosphere</i> , 2002, 47, 947-956.	8.2	59
48	An Update of the BCF QSAR Model Based on Theoretical Molecular Descriptors. <i>QSAR and Combinatorial Science</i> , 2005, 24, 953-960.	1.4	55
49	Are some "safer alternatives" hazardous as PBTs? The case study of new flame retardants. <i>Journal of Hazardous Materials</i> , 2016, 306, 237-246.	12.4	54
50	QSAR classification models for the prediction of endocrine disrupting activity of brominated flame retardants. <i>Journal of Hazardous Materials</i> , 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. <i>SAR and QSAR in Environmental Research</i> , 2006, 17, 265-284.	2.2	50
52	Aloeresin c, a bitter c,o-diglucoside from cape aloe. <i>Phytochemistry</i> , 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. <i>TrAC - Trends in Analytical Chemistry</i> , 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. <i>Environment International</i> , 2015, 77, 25-34.	10.0	48

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55	Ranking of aquatic toxicity of esters modelled by QSAR. <i>Chemosphere</i> , 2005, 58, 559-570.	8.2	47
56	QSAR study of malonyl-CoA decarboxylase inhibitors using GA-MLR and a new strategy of consensus modeling. <i>Journal of Computational Chemistry</i> , 2008, 29, 2636-2647.	3.3	46
57	Approaches for externally validated QSAR modelling of Nitrated Polycyclic Aromatic Hydrocarbon mutagenicity. <i>SAR and QSAR in Environmental Research</i> , 2007, 18, 169-178.	2.2	45
58	Screening the leaching tendency of pesticides applied in the Amu Darya Basin (Uzbekistan). <i>Water Research</i> , 2004, 38, 3485-3494.	11.3	44
59	A C-glucosylated 5-methylchromone from Kenya aloe. <i>Phytochemistry</i> , 1986, 25, 2219-2222.	2.9	43
60	QSAR Prediction of Ozone Tropospheric Degradation. <i>QSAR and Combinatorial Science</i> , 2003, 22, 364-373.	1.4	43
61	QSAR and Chemometric Approaches for Setting Water Quality Objectives for Dangerous Chemicals. <i>Ecotoxicology and Environmental Safety</i> , 2001, 49, 206-220.	6.0	42
62	Identification of potential PBT behavior of personal care products by structural approaches. <i>Sustainable Chemistry and Pharmacy</i> , 2015, 1, 19-27.	3.3	42
63	Stereoselective total synthesis of natural phytol double bond reductions by baker's yeast. <i>Tetrahedron</i> , 1987, 43, 4481-4486.	1.9	41
64	QSAR Modeling and Prediction of the Endocrine-Disrupting Potencies of Brominated Flame Retardants. <i>Chemical Research in Toxicology</i> , 2010, 23, 946-954.	3.3	41
65	In silico screening of estrogen-like chemicals based on different nonlinear classification models. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 26, 135-144.	2.4	38
66	The importance of molecular structures, endpoints <sup>TM</sup> values, and predictivity parameters in QSAR research: QSAR analysis of a series of estrogen receptor binders. <i>Molecular Diversity</i> , 2010, 14, 687-696.	3.9	38
67	Classification and Virtual Screening of Androgen Receptor Antagonists. <i>Journal of Chemical Information and Modeling</i> , 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).. <i>Tetrahedron Letters</i> , 1983, 24, 417-418.	1.4	36
69	Per- and Polyfluoro Toxicity (LC <sub>50</sub> Inhalation) Study in Rat and Mouse Using QSAR Modeling. <i>Chemical Research in Toxicology</i> , 2010, 23, 528-539.	3.3	35
70	Evaluation and QSAR modeling on multiple endpoints of estrogen activity based on different bioassays. <i>Chemosphere</i> , 2008, 70, 1889-1897.	8.2	34
71	QSAR modeling of cumulative environmental end-points for the prioritization of hazardous chemicals. <i>Environmental Sciences: Processes and Impacts</i> , 2018, 20, 38-47.	3.5	34
72	Steric Control of Conductivity in Highly Conjugated Polythiophenes. <i>Chemistry of Materials</i> , 2001, 13, 1665-1673.	6.7	33

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73	Accumulation of Persistent Organic Pollutants in Canopies of Different Forest Types: A Role of Species Composition and Altitudinal-Temperature Gradient. <i>Environmental Science &amp; Technology</i> , 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. <i>Atmospheric Environment</i> , 2014, 88, 212-218.	4.1	33
75	Prediction of PAH mutagenicity in human cells by QSAR classification. <i>SAR and QSAR in Environmental Research</i> , 2008, 19, 115-127.	2.2	32
76	CADASTER QSPR Models for Predictions of Melting and Boiling Points of Perfluorinated Chemicals. <i>Molecular Informatics</i> , 2011, 30, 189-204.	2.5	32
77	Modelling physico-chemical properties of (benzo)triazoles, and screening for environmental partitioning. <i>Water Research</i> , 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. <i>Tetrahedron Letters</i> , 1987, 28, 4221-4224.	1.4	30
79	Prediction of aromatic amines mutagenicity from theoretical molecular descriptors. <i>SAR and QSAR in Environmental Research</i> , 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. <i>Environmental Science and Pollution Research</i> , 2006, 13, 28-36.	5.3	29
81	QSAR classification of estrogen receptor binders and pre-screening of potential pleiotropic EDCs. <i>SAR and QSAR in Environmental Research</i> , 2010, 21, 657-669.	2.2	29
82	Oral LD50 toxicity modeling and prediction of per- and polyfluorinated chemicals on rat and mouse. <i>Molecular Diversity</i> , 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. <i>Food and Chemical Toxicology</i> , 2018, 112, 535-543.	3.6	27
85	Biosynthesis of phenylpropanoid compounds. Part I. Biosynthesis of eugenol in <i>Ocimum basilicum</i> L. <i>Journal of the Chemical Society Perkin Transactions 1</i> , 1974, , 1727.	0.9	26
86	Decarboxylation of cinnamic acids by <i>Saccharomyces cerevisiae</i> . <i>Bioorganic Chemistry</i> , 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. <i>Journal of Environmental Management</i> , 2008, 86, 419-426.	7.8	25
88	QSAR classification models for the screening of the endocrine-disrupting activity of perfluorinated compounds. <i>SAR and QSAR in Environmental Research</i> , 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. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 44, 266-277.	2.4	25
90	Synthesis, photodynamic activity, and quantitative structure-activity relationship modelling of a series of BODIPYs. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2017, 167, 269-281.	3.8	25

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91	BAKER'S YEAST HYDROGENATION OF CARBONYL ACTIVATED DOUBLE BONDS. ENANTIOSELECTIVE SYNTHESIS OF THE (S)-FORM OF THE DIHYDROTERPENEDIOL SECRETED BY DANAUS CHRYSIPPUS AND OF A PHEROMONE OF CALLOSOBROCHUS CHINENSIS. <i>Chemistry Letters</i> , 1985, 14, 1395-1398.	1.3	24
92	Prediction of infinite-dilution activity coefficients of organic solutes in ionic liquids using temperature-dependent quantitative structure-property relationship method. <i>Chemical Engineering Journal</i> , 2010, 163, 195-201.	12.7	24
93	Screening of persistent organic pollutants by QSPR classification models: A comparative study. <i>Journal of Molecular Graphics and Modelling</i> , 2008, 27, 59-65.	2.4	23
94	Externally validated QSPR modelling of VOC tropospheric oxidation by NO <sub>3</sub> radicals. <i>SAR and QSAR in Environmental Research</i> , 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. <i>Atmospheric Environment</i> , 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 amiprofos methyl. <i>Medicinal Chemistry Research</i> , 2014, 23, 4825-4835.	2.4	22
97	QSAR prediction of the competitive interaction of emerging halogenated pollutants with human transthyretin. <i>SAR and QSAR in Environmental Research</i> , 2013, 24, 333-349.	2.2	21
98	WHIM Descriptors of Shape. <i>QSAR and Combinatorial Science</i> , 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. <i>Tetrahedron Letters</i> , 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. <i>ATLA Alternatives To Laboratory Animals</i> , 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. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2010, , 327-366.	0.6	17
102	Quantitative structure-activity relationship modeling of polycyclic aromatic hydrocarbon mutagenicity by classification methods based on holistic theoretical molecular descriptors. <i>Ecotoxicology and Environmental Safety</i> , 2007, 66, 353-361.	6.0	16
103	QSPRINS - Chem standalone version: A new platform-independent software to profile chemicals for physicochemical properties, fate, and toxicity. <i>Journal of Computational Chemistry</i> , 2021, 42, 1452-1460.	3.3	16
104	Modeling ready biodegradability of fragrance materials. <i>Environmental Toxicology and Chemistry</i> , 2015, 34, 1224-1231.	4.3	15
105	Quantitative structure-activity relationship modelling of oral acute toxicity and cytotoxic activity of fragrance materials in rodents. <i>SAR and QSAR in Environmental Research</i> , 2009, 20, 767-779.	2.2	14
106	The Applications of Machine Learning Algorithms in the Modeling of Estrogen-Like Chemicals. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2009, 12, 490-496.	1.1	14
107	On the Use of Local and Global QSPRs for the Prediction of Physicochemical Properties of Polybrominated Diphenyl Ethers. <i>Molecular Informatics</i> , 2011, 30, 232-240.	2.5	14
108	Reduction of cinnamyl alcohols and cinnamaldehydes by <i>Saccharomyces cerevisiae</i> . <i>Bioorganic Chemistry</i> , 1981, 10, 22-28.	4.1	13

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109	In Memory of Professor Davide Calamari. <i>Environmental Science and Pollution Research</i> , 2006, 13, 1-1.	5.3	13
110	Stereochemistry of the decarboxylation of phenolic cinnamic acids by <i>Saccharomyces cerevisiae</i> . <i>Journal of the Chemical Society Chemical Communications</i> , 1975, , 442.	2.0	12
111	Ranking and classification of non-ionic organic pesticides for environmental distribution: a qsar approach. <i>International Journal of Environmental Analytical Chemistry</i> , 2004, 84, 65-74.	3.3	11
112	Are Mechanistic and Statistical QSAR Approaches Really Different? MLR Studies on 158 Cycloalkylâ€Pyranones. <i>Molecular Informatics</i> , 2010, 29, 511-522.	2.5	11
113	Biosynthesis of anethole in <i>L.</i> <i>Tetrahedron Letters</i> , 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. <i>ATLA Alternatives To Laboratory Animals</i> , 2014, 42, 13-24.	1.0	10
116	A Combined Quantitative Structure-Activity Relationship Research of Quinolinone Derivatives as Androgen Receptor Antagonists. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2015, 18, 834-845.	1.1	10
117	Multivariate Chemical Mapping of Antibiotics and Identification of Structurally Representative Substances. <i>Environmental Science &amp; Technology</i> , 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. <i>Journal of the Chemical Society Chemical Communications</i> , 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. <i>Bioconjugate Chemistry</i> , 1999, 10, 332-337.	3.6	7
121	Combined Ligand/Structure-Based Virtual Screening and Molecular Dynamics Simulations of Steroidal Androgen Receptor Antagonists. <i>BioMed Research International</i> , 2017, 2017, 1-18.	1.9	7
122	Synthesis of (2S, 5R) - [5-2H] Proline. <i>Journal of Labelled Compounds and Radiopharmaceuticals</i> , 1981, 18, 955-962.	1.0	6
123	Structureâ€Activity Relationship Analysis of the Thermal Stabilities of Nitroaromatic Compounds Following Different Decomposition Mechanisms. <i>Molecular Informatics</i> , 2013, 32, 193-202.	2.5	5
124	Ligand Efficiency Outperforms $plC_{50}$ on Both 2D $MLR$ and 3D $CoMFA$ Models: A Case Study on $AR$ Antagonists. <i>Chemical Biology and Drug Design</i> , 2015, 86, 1501-1517.	3.2	5
125	Ranking of Phenols for Abiotic Oxidation in Aqueous Environment: a QSPR Approach. <i>Annali Di Chimica</i> , 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. <i>Journal of Computational Chemistry</i> , 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 "QSAR model reproducibility and applicability: A case study of rate constants of hydroxyl radical reaction models applied to polybrominated diphenyl ethers and (benzo)triazoles", 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 structure-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