Roberto Todeschini

List of Publications by Year
in descending order

181 papers	13,980 citations	57758 44 h-index	21540 114 g-index
213 all docs	213 docs citations	213 times ranked	11355 citing authors

#	ARTICLE	IF	CITATIONS
1	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	6.4	1,401
2	Virtual Computational Chemistry Laboratory – Design and Description. Journal of Computer-Aided Molecular Design, 2005, 19, 453-463.	2.9	1,250
3	Comments on the Definition of the Q^2 Parameter for QSAR Validation. Journal of Chemical Information and Modeling, 2009, 49, 1669-1678.	5.4	483
4	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Computer-Aided Molecular Design, 2011, 25, 533-554.	2.9	453
5	Structure/Response Correlations and Similarity/Diversity Analysis by GETAWAY Descriptors. 1. Theory of the Novel 3D Molecular Descriptors. Journal of Chemical Information and Computer Sciences, 2002, 42, 682-692.	2.8	402
6	Comparison of Different Approaches to Define the Applicability Domain of QSAR Models. Molecules, 2012, 17, 4791-4810.	3.8	370
7	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
8	Evaluation of model predictive ability by external validation techniques. Journal of Chemometrics, 2010, 24, 194-201.	1.3	290
9	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
10	New molecular descriptors for 2D and 3D structures. Theory. Journal of Chemometrics, 1994, 8, 263-272.	1.3	269
11	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	6.0	264
12	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
13	Multivariate comparison of classification performance measures. Chemometrics and Intelligent Laboratory Systems, 2018, 174, 33-44.	3.5	195
14	The K correlation index: theory development and its application in chemometrics. Chemometrics and Intelligent Laboratory Systems, 1999, 46, 13-29.	3.5	172
15	Quantitative Structure–Activity Relationship Models for Ready Biodegradability of Chemicals. Journal of Chemical Information and Modeling, 2013, 53, 867-878.	5.4	160
16	Detecting "bad" regression models: multicriteria fitness functions in regression analysis. Analytica Chimica Acta, 2004, 515, 199-208.	5.4	156
17	Similarity Coefficients for Binary Chemoinformatics Data: Overview and Extended Comparison Using Simulated and Real Data Sets. Journal of Chemical Information and Modeling, 2012, 52, 2884-2901.	5.4	155
18	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

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19	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
20	The BEAM-project: prediction and assessment of mixture toxicities in the aquatic environment. Continental Shelf Research, 2003, 23, 1757-1769.	1.8	111
21	The Kohonen and CP-ANN toolbox: A collection of MATLAB modules for Self Organizing Maps and Counterpropagation Artificial Neural Networks. Chemometrics and Intelligent Laboratory Systems, 2009, 98, 115-122.	3.5	111
22	A new algorithm for optimal, distance-based experimental design. Chemometrics and Intelligent Laboratory Systems, 1992, 16, 37-44.	3.5	99
23	MS-WHIM, new 3D theoretical descriptors derived from molecular surface properties: a comparative 3D QSAR study in a series of steroids. Journal of Computer-Aided Molecular Design, 1997, 11, 79-92.	2.9	96
24	Lewis acid mediated aldol condensations using thioester silyl ketene acetals. Tetrahedron, 1986, 42, 893-909.	1.9	87
25	Weighted holistic invariant molecular descriptors. Part 2. Theory development and applications on modeling physicochemical properties of polyaromatic hydrocarbons. Chemometrics and Intelligent Laboratory Systems, 1995, 27, 221-229.	3.5	84
26	Beware of Unreliable Q^2! A Comparative Study of Regression Metrics for Predictivity Assessment of QSAR Models. Journal of Chemical Information and Modeling, 2016, 56, 1905-1913.	5.4	84
27	3D-modelling and prediction by WHIM descriptors. Part 9. Chromatographic relative retention time and physico-chemical properties of polychlorinated biphenyls (PCBs). Chemometrics and Intelligent Laboratory Systems, 1998, 40, 53-63.	3.5	81
28	The Whim Theory: New 3D Molecular Descriptors for Qsar in Environmental Modelling. SAR and QSAR in Environmental Research, 1997, 7, 89-115.	2.2	80
29	New 3D molecular descriptors: the WHIM theory and QSAR applications. Journal of Computer - Aided Molecular Design, 1998, 9/11, 355-380.	1.0	71
30	QSAR study on the tropospheric degradation of organic compounds. Chemosphere, 1999, 38, 1371-1378.	8.2	67
31	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
32	Defining a novel k-nearest neighbours approach to assess the applicability domain of a QSAR model for reliable predictions. Journal of Cheminformatics, 2013, 5, 27.	6.1	65
33	Modeling and prediction by using whim descriptors in QSAR studies: toxicity of heterogeneous chemicals on Daphnia magna. Chemosphere, 1996, 32, 1527-1545.	8.2	64
34	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
35	Data correlation, number of significant principal components and shape of molecules. The K correlation index. Analytica Chimica Acta, 1997, 348, 419-430.	5.4	62
36	Molecular Descriptors. Challenges and Advances in Computational Chemistry and Physics, 2010, , 29-102.	0.6	62

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37	Locally centred Mahalanobis distance: A new distance measure with salient features towards outlier detection. Analytica Chimica Acta, 2013, 787, 1-9.	5.4	60
38	A novel variable reduction method adapted from space-filling designs. Chemometrics and Intelligent Laboratory Systems, 2014, 136, 147-154.	3.5	60
39	Prediction of Acute Aquatic Toxicity toward *Daphnia Magna* by using the GA-*k*NN Method. ATLA Alternatives To Laboratory Animals, 2014, 42, 31-41.	1.0	59
40	Multivariate Classification for Qualitative Analysis. , 2009, , 83-104.		50
41	A similarity-based QSAR model for predicting acute toxicity towards the fathead minnow (*Pimephales promelas*). SAR and QSAR in Environmental Research, 2015, 26, 217-243.	2.2	50
42	In Silico Prediction of Cytochrome P450-Drug Interaction: QSARs for CYP3A4 and CYP2C9. International Journal of Molecular Sciences, 2016, 17, 914.	4.1	50
43	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
44	Kohonen artificial neural networks as a tool for wavelength selection in multicomponent spectrofluorimetric PLS modelling: application to phenol, o-cresol, m-cresol and p-cresol mixtures. TrAC - Trends in Analytical Chemistry, 1999, 18, 93-98.	11.4	45
45	QSAR and Chemometric Approaches for Setting Water Quality Objectives for Dangerous Chemicals. Ecotoxicology and Environmental Safety, 2001, 49, 206-220.	6.0	42
46	Scaffold hopping from natural products to synthetic mimetics by holistic molecular similarity. Communications Chemistry, 2018, 1, .	4.5	42
47	Modeling and prediction by using WHIM descriptors in QSAR studies: submitochondrial particles (SMP) as toxicity biosensors of chlorophenols. Chemosphere, 1996, 33, 71-79.	8.2	41
48	QSAR approach for the selection of congeneric compounds with a similar toxicological mode of action. Chemosphere, 2001, 42, 873-883.	8.2	41
49	QSAR models for bioconcentration: Is the increase in the complexity justified by more accurate predictions?. Chemosphere, 2015, 127, 171-179.	8.2	41
50	A QSTR-Based Expert System to Predict Sweetness of Molecules. Frontiers in Chemistry, 2017, 5, 53.	3.6	41
51	Weighted holistic invariant molecular descriptors. Part 2. Theory development and applications on modeling physicochemical properties of polyaromatic hydrocarbons. Chemometrics and Intelligent Laboratory Systems, 1995, 27, 221-229.	3.5	41
52	30-Modelling and Prediction by WHIM Descriptors. Part 8. Toxicity and Physico-chemical Properties of Environmental Priority Chemicals by 2D-TI and 3D-WHIM Descriptors. SAR and QSAR in Environmental Research, 1997, 7, 173-193.	2.2	40
53	CAIMAN (Classification And Influence Matrix Analysis): A new approach to the classification based on leverage-scaled functions. Chemometrics and Intelligent Laboratory Systems, 2007, 87, 3-17.	3.5	39
54	Chemometric optimization of the ruthenium carbonyl catalysed cyclization of 2-nitrostilbene to 2-phenylindole. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 2811.	1.7	38

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55	Submitochondrial particles as toxicity biosensors of chlorophenols. Environmental Toxicology and Chemistry, 1995, 14, 363-368.	4.3	38
56	Chemometrics in QSAR. , 2009, , 129-172.		38
57	Sensitivity assessment of freshwater macroinvertebrates to pesticides using biological traits. Ecotoxicology, 2012, 21, 336-352.	2.4	37
58	Geographical identification of Chianti red wine based on ICP-MS element composition. Food Chemistry, 2020, 315, 126248.	8.2	37
59	Theoretical studies of stereoselective aldol condensations. Journal of Organic Chemistry, 1986, 51, 612-616.	3.2	36
60	Towards Global QSAR Model Building for Acute Toxicity: Munro Database Case Study. International Journal of Molecular Sciences, 2014, 15, 18162-18174.	4.1	36
61	The chemical meaning of topological indices. Chemometrics and Intelligent Laboratory Systems, 1992, 15, 51-59.	3.5	35
62	MobyDigs: software for regression and classification models by genetic algorithms. Data Handling in Science and Technology, 2003, 23, 141-167.	3.1	34
63	Impact of Molecular Descriptors on Computational Models. Methods in Molecular Biology, 2018, 1825, 171-209.	0.9	34
64	Steric Control of Conductivity in Highly Conjugated Polythiophenes. Chemistry of Materials, 2001, 13, 1665-1673.	6.7	33
65	N3 and BNN: Two New Similarity Based Classification Methods in Comparison with Other Classifiers. Journal of Chemical Information and Modeling, 2015, 55, 2365-2374.	5.4	32
66	Investigating the mechanisms of bioconcentration through QSAR classification trees. Environment International, 2016, 88, 198-205.	10.0	32
67	On the Misleading Use of for QSAR Model Comparison. Molecular Informatics, 2019, 38, e1800029.	2.5	31
68	New indices for analysing partial ranking diagrams. Analytica Chimica Acta, 2004, 515, 167-181.	5.4	30
69	Molecular Descriptors. , 2017, , 2065-2093.		30
70	Integrated QSAR Models to Predict Acute Oral Systemic Toxicity. Molecular Informatics, 2019, 38, e1800124.	2.5	30
71	Rabbit nest construction and its relationship with litter development. Applied Animal Behaviour Science, 1991, 31, 259-266.	1.9	29
72	Multicriteria Decision-Making Methods. , 2009, , 591-629.		29

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73	The j-index: a new bibliometric index and multivariate comparisons between other common indices. Scientometrics, 2011, 87, 621-639.	3.0	29
74	New 3D Molecular Descriptors: The WHIM theory and QSAR Applications. , 2002, , 355-380.		28
75	A distance measure between models: a tool for similarity/diversity analysis of model populations. Chemometrics and Intelligent Laboratory Systems, 2004, 70, 55-61.	3.5	28
76	Assessing bioaccumulation of polybrominated diphenyl ethers for aquatic species by QSAR modeling. Chemosphere, 2012, 89, 433-444.	8.2	28
77	Molecular Descriptors for Structure–Activity Applications: A Hands-On Approach. Methods in Molecular Biology, 2018, 1800, 3-53.	0.9	28
78	Stereoselective aldol condensations via alkenyloxy dialkoxyboranes : mechanistic and stereochemical details. Tetrahedron, 1984, 40, 4051-4058.	1.9	27
79	Traditional versus WHIM molecular descriptors in QSAR approaches applied to fish toxicity studies. Chemosphere, 2001, 44, 401-406.	8.2	27
80	Geographical classification of wine and olive oil by means of classification and influence matrix analysis (CAIMAN). Analytica Chimica Acta, 2006, 570, 249-258.	5.4	27
81	A new concept of higher-order similarity and the role of distance/similarity measures in local classification methods. Chemometrics and Intelligent Laboratory Systems, 2016, 157, 50-57.	3.5	27
82	Quantitative structure–activity relationships to predict sweet and non-sweet tastes. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	27
83	Application of the Kohonen artificial neural network in the identification of proteinaceous binders in samples of panel painting using gas chromatography-mass spectrometry. Analyst, The, 2003, 128, 281-286.	3.5	26
84	k-nearest neighbour method: The influence of data transformations and metrics. Chemometrics and Intelligent Laboratory Systems, 1989, 6, 213-220.	3.5	25
85	Study on anaerobic and aerobic degradation of different non-ionic surfactants. Bioresource Technology, 2003, 87, 87-91.	9.6	25
86	Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 1. Theory and simple chemometric applications. Analytica Chimica Acta, 2009, 648, 45-51.	5.4	25
87	Expert QSAR system for predicting the bioconcentration factor under the REACH regulation. Environmental Research, 2016, 148, 507-512.	7.5	24
88	Assessing the Validity of QSARs for Ready Biodegradability of Chemicals: An Applicability Domain Perspective. Current Computer-Aided Drug Design, 2014, 10, 137-147.	1.2	24
89	Modeling and prediction of molecular properties. Theory of grid-weighted holistic invariant molecular (G-WHIM) descriptors. Chemometrics and Intelligent Laboratory Systems, 1997, 36, 65-73.	3.5	23
90	Characterization of the traditional Cypriot spirit Zivania by means of Counterpropagation Artificial Neural Networks. Chemometrics and Intelligent Laboratory Systems, 2007, 87, 52-58.	3.5	23

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91	The combustion of municipal solid wastes and PCDD and PCDF emissions. Part 2. PCDD and PCDF in stack gases. Chemosphere, 1989, 18, 1465-1474.	8.2	22
92	A chemometric approach based on a novel similarity/diversity measure for the characterisation and selection of electronic nose sensors. Analytica Chimica Acta, 2006, 578, 170-177.	5.4	22
93	A MATLAB toolbox for multivariate regression coupled with variable selection. Chemometrics and Intelligent Laboratory Systems, 2021, 213, 104313.	3.5	22
94	K-CM: A new artificial neural network. Application to supervised pattern recognition. Chemometrics and Intelligent Laboratory Systems, 2014, 138, 110-119.	3.5	20
95	Recent Advances in High-Level Fusion Methods to Classify Multiple Analytical Chemical Data. Data Handling in Science and Technology, 2019, 31, 129-155.	3.1	19
96	Geometry and energy of overcrowded ethylenes. II. Bornanylidene, fenchylidene, and bifluorenylidene derivatives. Journal of Computational Chemistry, 1982, 3, 178-184.	3.3	18
97	Matrixâ€based Molecular Descriptors for Prospective Virtual Compound Screening. Molecular Informatics, 2017, 36, 1600091.	2.5	18
98	Classification of multiway analytical data based on MOLMAP approach. Analytica Chimica Acta, 2007, 605, 134-146.	5.4	17
99	Reshaped Sequential Replacement algorithm: An efficient approach to variable selection. Chemometrics and Intelligent Laboratory Systems, 2014, 133, 136-148.	3.5	17
100	Molecular conformation of cyclenes. Journal of Molecular Structure, 1977, 41, 305-313.	3.6	15
101	Geometry and energy of tetra-tert-butylethylene. Journal of Computational Chemistry, 1981, 2, 149-156.	3.3	15
102	Pharmacophore Identification in Amnesia-Reversal Compounds Using Conformational Analysis and Chemometric Methods. QSAR and Combinatorial Science, 1990, 9, 195-201.	1.2	15
103	A fast method for the calculation of partial least squares coefficients. Chemometrics and Intelligent Laboratory Systems, 1991, 12, 117-120.	3.5	15
104	Linear discriminant classification tree: A user-driven multicriteria classification method. Chemometrics and Intelligent Laboratory Systems, 1992, 16, 25-35.	3.5	15
105	A 3D QSAR approach to the search for geometrical similarity in a series of nonpeptide angiotensin II receptor antagonists. Journal of Computer-Aided Molecular Design, 1994, 8, 211-220.	2.9	15
106	Chemometric analysis of gas chromatography with flame ionisation detection chromatograms: A novel method for classification of petroleum products. Journal of Chromatography A, 2012, 1238, 121-127.	3.7	15
107	Reshaped <scp>Sequential Replacement</scp> for variable selection in QSPR: comparison with other reference methods. Journal of Chemometrics, 2014, 28, 249-259.	1.3	15
108	A theoretical conformational study of pushâ€"pull ethylenes. Part 1. Substituted methyleneimidazolidines. Journal of the Chemical Society Perkin Transactions II, 1985, , 915-920.	0.9	14

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109	Total ranking models by the genetic algorithm variable subset selection (GA?VSS) approach for environmental priority settings. Analytical and Bioanalytical Chemistry, 2004, 380, 430-444.	3.7	14
110	Qualitative consensus of QSAR ready biodegradability predictions. Toxicological and Environmental Chemistry, 0, , 1-24.	1.2	14
111	The combustion of municipal solid wastes and PCDD and PCDF emissions. Part 1. PCDD and PCDF in MSW. Chemosphere, 1989, 18, 1457-1464.	8.2	13
112	The combustion of municipal solid wastes: PCDD and PCDF in MSW and in emissions. A chemometric approach. Chemosphere, 1989, 19, 751-757.	8.2	13
113	Pharmacophore identification by molecular modeling and chemometrics: The case of HMG-CoA reductase inhibitors. Journal of Computer-Aided Molecular Design, 1992, 6, 47-60.	2.9	13
114	3D-Modelling and Prediction by Whim Descriptors. Part 7. Physico-Chemical Properties of Haloaromatics: Comparison Between Whim and Topological Descriptors. SAR and QSAR in Environmental Research, 1997, 7, 133-150.	2.2	13
115	Characterization of DNA Primary Sequences by a New Similarity/Diversity Measure Based on the Partial Ordering. Journal of Chemical Information and Modeling, 2006, 46, 1905-1911.	5.4	13
116	Self Organizing Maps for Analysis of Polycyclic Aromatic Hydrocarbons 3-Way Data from Spilled Oils. Analytical Chemistry, 2010, 82, 4264-4271.	6.5	13
117	Weighted power–weakness ratio for multi-criteria decision making. Chemometrics and Intelligent Laboratory Systems, 2015, 146, 329-336.	3.5	13
118	Predicting molecular activity on nuclear receptors by multitask neural networks. Journal of Chemometrics, 2022, 36, e3325.	1.3	13
119	Molecular Descriptors. , 2016, , 1-29.		13
120	The molecular structure of vinyl azide. Journal of Molecular Structure, 1978, 50, 191-193.	3.6	12
121	Conformational analysis of polysubstituted ethanes. Journal of the American Chemical Society, 1981, 103, 3679-3682.	13.7	12
122	The combustion of municipal solid wastes and PCDD and PCDF emissions. Part 3. PCDD and PCDF in fly ash. Chemosphere, 1989, 18, 1475-1483.	8.2	12
123	How to weight Hasse matrices and reduce incomparabilities. Chemometrics and Intelligent Laboratory Systems, 2015, 147, 95-104.	3.5	12
124	Conformation of bicyclo[n.1.0]-compounds. Journal of Molecular Structure, 1980, 64, 47-55.	3.6	11
125	Conformation of bicyclo[n.1.0] derivatives. Journal of Molecular Structure, 1981, 71, 279-286.	3.6	11
126	Conformation of bicyclo [n.1.0] Derivatives. Computational and Theoretical Chemistry, 1982, 87, 53-64.	1.5	11

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127	Weighted k-Nearest Neighbour Method for the Calculation of Missing Values. Chemometrics and Intelligent Laboratory Systems, 1990, 9, 201-205.	3.5	11
128	Hydroxylamine-Induced Cleavage of the Asparaginylâ€"Glycine Motif in the Production of Recombinant Proteins: The Case of Insulin-like Growth Factor I. Protein Expression and Purification, 1997, 11, 135-147.	1.3	11
129	Response surface models for the formation of PCDD and PCDF in a pilot plant combustion of MSW. Chemosphere, 1990, 20, 1973-1979.	8.2	10
130	Mixtures, metabolites, ionic liquids: a new measure to evaluate similarity between complex chemical systems. Journal of Cheminformatics, 2016, 8, 49.	6.1	10
131	Parsimonious Optimization of Multitask Neural Network Hyperparameters. Molecules, 2021, 26, 7254.	3.8	10
132	CONFORMATIONAL ANALYSIS OF TRIMETHYLPHOSPHITE AND ITS METAL COMPLEXES. Phosphorous and Sulfur and the Related Elements, 1983, 17, 205-220.	0.2	9
133	PCDD and PCDF in emissions from the combustion of MSW in a pilot plant. Preliminary results. Chemosphere, 1989, 19, 417-422.	8.2	9
134	Linear discriminant hierarchical clustering: A modeling and cross-validable divisive clustering method. Chemometrics and Intelligent Laboratory Systems, 1993, 19, 43-51.	3.5	9
135	Chapter 2 Total-Order Ranking Methods. Data Handling in Science and Technology, 2008, 27, 51-72.	3.1	9
136	Empirical force field calculations for bridged annulenes. Journal of Chemical Physics, 1981, 74, 3953-3960.	3.0	8
137	Structure-activity relationship of Ca2+ channel blockers: A study using conformational analysis and chemometric methods. Journal of Computer-Aided Molecular Design, 1991, 5, 571-584.	2.9	8
138	Hybrid toxicology expert system: architecture and implementation of a multi-domain hybrid expert system for toxicology. Chemometrics and Intelligent Laboratory Systems, 1998, 43, 135-145.	3.5	8
139	A combined use of global and local approaches in 3D-QSAR. Chemometrics and Intelligent Laboratory Systems, 2000, 52, 183-194.	3.5	8
140	New QSAR Modelling Approach Based on Ranking Models by Genetic Algorithms - Variable Subset Selection (GA-VSS). , 2006, , 181-217.		8
141	Data Mining by Total Ranking Methods: A Case Study on Optimisation of the â€œPulp and Bleachingâ€• Process in the Paper Industry. Annali Di Chimica, 2006, 96, 13-27.	0.6	8
142	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
143	Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Analytica Chimica Acta, 2009, 648, 52-59.	5.4	7
144	Canonical Measure of Correlation (CMC) and Canonical Measure of Distance (CMD) between sets of data. Part 3. Variable selection in classification. Analytica Chimica Acta, 2010, 657, 116-122.	5.4	7

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145	QSPR STUDY OF RHEOLOGICAL AND MECHANICAL PROPERTIES OF CHLOROPRENE RUBBER ACCELERATORS. Rubber Chemistry and Technology, 2014, 87, 219-238.	1.2	7
146	Classification-based QSAR Models for the Prediction of the Bioactivity of ACE-inhibitor Peptides. Protein and Peptide Letters, 2018, 25, 1015-1023.	0.9	7
147	Chapter 9 The DART (Decision Analysis by Ranking Techniques) Software. Data Handling in Science and Technology, 2008, , 193-207.	3.1	6
148	Deep Ranking Analysis by Power Eigenvectors (DRAPE): A wizard for ranking and multi-criteria decision making. Chemometrics and Intelligent Laboratory Systems, 2019, 191, 129-137.	3.5	6
149	Chemometrics for QSAR Modeling. , 2020, , 599-634.		6
150	Molecular structure of strained polycyclic hydrocarbons. A MINDO/3 study of some bicyclo- and tricyclo-derivatives. Journal of Molecular Structure, 1979, 53, 267-273.	3.6	5
151	Chemometric approaches in environmental problems concerning PCDD and PCDF. Data interpretation and source correlation. Mechanisms of formation and destruction in MSW combustion process. Fresenius' Journal of Analytical Chemistry, 1994, 348, 111-120.	1.5	5
152	Conformation of bicyclo[n.1.0] derivatives. Journal of Molecular Structure, 1982, 90, 165-176.	3.6	4
153	Empirical force field calculations for bridged annulenes. II. 1,6â€ethanoâ€8,13â€methanoâ€and 1,6:7,12â€bismethanoâ€â€"14â€"annulenes. Journal of Chemical Physics, 1983, 78, 1895-1897.	3.0	4
154	A chemometric approach for evaluating the efficiency of a pilot plant for MSW combustion. Chemosphere, 1991, 23, 1407-1416.	8.2	4
155	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Cheminformatics, 2011, 3, .	6.1	4
156	Structure â€"Activity Relationships by Autocorrelation Descriptors and Genetic Algorithms. , 2011, , 60-94.		4
157	Conformation of bicyclo [n.1.0] derivatives. Computational and Theoretical Chemistry, 1982, 90, 165-176.	1.5	3
158	Multicriteria Decision-Making Methods. , 2009, , 585-615.		3
159	Dairy cream response in instrumental texture evaluation processed by multivariate analysis. Chemometrics and Intelligent Laboratory Systems, 2009, 96, 258-263.	3.5	3
160	Experimental and Theoretical Studies in the EU FP7 Marie Curie Initial Training Network Project, Environmental ChemOinformatics (ECO). ATLA Alternatives To Laboratory Animals, 2014, 42, 7-11.	1.0	3
161	Data Analysis in Chemistry and Bio-Medical Sciences. International Journal of Molecular Sciences, 2016, 17, 2105.	4.1	3
162	Principal Component Analysis to interpret changes in chromatic parameters on paint dosimeters exposed long-term to urban air. Chemometrics and Intelligent Laboratory Systems, 2017, 167, 113-122.	3.5	3

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163	Crystal, molecular, and electronic structure of 13,13-difluoro-1,7-methano[12]annulene. Journal of the Chemical Society Perkin Transactions II, 1983, , 1227.	0.9	2
164	Conformation of bicyclo [n.1.0] derivatives. Computational and Theoretical Chemistry, 1983, 105, 17-29.	1.5	2
165	Methodologies for the identification of the pharmacophore in series of bioactive compounds. Journal of Molecular Graphics, 1991, 9, 70.	1.1	2
166	Factors affecting cytochrome P-450 and horseradish peroxidase-catalyzed oxidative N-dealkylation of aromatic tertiary amines. A multivariate approach. Journal of Molecular Catalysis, 1993, 85, 97-108.	1.2	2
167	Deep Ranking Analysis by Power Eigenvectors (DRAPE): A polypharmacology case study. Chemometrics and Intelligent Laboratory Systems, 2020, 203, 104001.	3.5	2
168	Resolution of mixtures of three nonsteroidal anti-inflammatory drugs by fluorescence using partial least squares multivariate calibration with previous wavelength selection by Kohonen artificial neural networks. Talanta, 2000, 52, 1069-79.	5.5	2
169	Electro-optical properties of the oxirane skeleton and the carbon–carbon bond in its derivatives. Journal of the Chemical Society Faraday Transactions I, 1981, 77, 1611.	1.0	1
170	The conformation of 1-vinylcyclohexene. Computational and Theoretical Chemistry, 1983, 105, 291-306.	1.5	1
171	Conformational studies of octalene and its benzo-derivatives. Journal of Computational Chemistry, 1984, 5, 343-348.	3.3	1
172	Mapping of Activity through Dichotomic Scores (MADS): A new chemoinformatic approach to detect activity–rich structural regions. Journal of Chemometrics, 2018, 32, e2994.	1.3	1
173	Chemometrics for Sampling and Analysis: Theory and Environmental Applications. , 2000, , 387-404.		1
174	Determination of platinum in plasma of patients affected by inoperable lung carcinoma treated with radiotherapy and concurrent low-dose continuous infusion of cis-dichlorodiammine platinum(II). Cancer Chemotherapy and Pharmacology, 1995, 35, 529-532.	2.3	1
175	School of Chemometrics, Cuenca, Ecuador, 8–12 May 1989. Chemometrics and Intelligent Laboratory Systems, 1989, 6, 258.	3.5	0
176	A new procedure for the visual inspection of multivariate data of different geographic origins. Chemometrics and Intelligent Laboratory Systems, 1991, 12, 181-187.	3.5	0
177	Steric effects in polybitniophenes. , 1994, , .		0
178	Geographical Characterization of Olive Oil by Means of Multivariate Classification. , 2010, , 129-137.		0
179	A New Molecular Structure Representation: Spectral Weighted Molecular (SWM) Signals and Spectral Weighted Invariant Molecular (SWIM) Descriptors. , 2000, , 344-344.		0
180	QSAR Approach for the Selection of Congeneric Compounds with Similar Toxicological Modes of Action. , 2000, , 292-292.		0

#	ARTICLE	IF	CITATIONS
181	Abstract OT3-02-05: Phase II study of eribulin in combination with gemcitabine for the treatment of patients with locally advanced or metastatic triple negative breast cancer. ERIGE Trial on behalf of the Gruppo Oncologico Italiano di Ricerca Clinica (GOIRC). , 2016, , .		0