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	Predicting molecular activity on nuclear receptors by multitask neural networks. Journal of Chemometrics, 2022, 36, e3325.	1.3	13
2	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
3	A MATLAB toolbox for multivariate regression coupled with variable selection. Chemometrics and Intelligent Laboratory Systems, 2021, 213, 104313.	3.5	22
4	Parsimonious Optimization of Multitask Neural Network Hyperparameters. Molecules, 2021, 26, 7254.	3.8	10
5	Chemometrics for QSAR Modeling. , 2020, , 599-634.		6
6	Deep Ranking Analysis by Power Eigenvectors (DRAPE): A polypharmacology case study. Chemometrics and Intelligent Laboratory Systems, 2020, 203, 104001.	3.5	2
7	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
8	Geographical identification of Chianti red wine based on ICP-MS element composition. Food Chemistry, 2020, 315, 126248.	8.2	37
9	On the Misleading Use of for QSAR Model Comparison. Molecular Informatics, 2019, 38, e1800029.	2.5	31
10	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
11	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
12	Integrated QSAR Models to Predict Acute Oral Systemic Toxicity. Molecular Informatics, 2019, 38, e1800124.	2.5	30
13	Mapping of Activity through Dichotomic Scores (MADS): A new chemoinformatic approach to detect activityâ€rich structural regions. Journal of Chemometrics, 2018, 32, e2994.	1.3	1
14	Multivariate comparison of classification performance measures. Chemometrics and Intelligent Laboratory Systems, 2018, 174, 33-44.	3.5	195
15	Impact of Molecular Descriptors on Computational Models. Methods in Molecular Biology, 2018, 1825, 171-209.	0.9	34
16	Molecular Descriptors for Structureâ€“Activity Applications: A Hands-On Approach. Methods in Molecular Biology, 2018, 1800, 3-53.	0.9	28
17	Scaffold hopping from natural products to synthetic mimetics by holistic molecular similarity. Communications Chemistry, 2018, 1, .	4.5	42
18	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

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19	Molecular Descriptors. , 2017, , 2065-2093.		30
20	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
21	Matrixâ€based Molecular Descriptors for Prospective Virtual Compound Screening. Molecular Informatics, 2017, 36, 1600091.	2.5	18
22	A QSTR-Based Expert System to Predict Sweetness of Molecules. Frontiers in Chemistry, 2017, 5, 53.	3.6	41
23	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	6.0	264
24	In Silico Prediction of Cytochrome P450-Drug Interaction: QSARs for CYP3A4 and CYP2C9. International Journal of Molecular Sciences, 2016, 17, 914.	4.1	50
25	Data Analysis in Chemistry and Bio-Medical Sciences. International Journal of Molecular Sciences, 2016, 17, 2105.	4.1	3
26	Expert QSAR system for predicting the bioconcentration factor under the REACH regulation. Environmental Research, 2016, 148, 507-512.	7.5	24
27	Beware of Unreliable Q²! 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
28	Mixtures, metabolites, ionic liquids: a new measure to evaluate similarity between complex chemical systems. Journal of Cheminformatics, 2016, 8, 49.	6.1	10
29	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
30	Quantitative structureâ€“activity relationships to predict sweet and non-sweet tastes. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	27
31	Investigating the mechanisms of bioconcentration through QSAR classification trees. Environment International, 2016, 88, 198-205.	10.0	32
32	Molecular Descriptors. , 2016, , 1-29.		13
33	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
34	QSAR models for bioconcentration: Is the increase in the complexity justified by more accurate predictions?. Chemosphere, 2015, 127, 171-179.	8.2	41
35	Weighted powerâ€“weakness ratio for multi-criteria decision making. Chemometrics and Intelligent Laboratory Systems, 2015, 146, 329-336.	3.5	13
36	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

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37	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
38	How to weight Hasse matrices and reduce incomparabilities. Chemometrics and Intelligent Laboratory Systems, 2015, 147, 95-104.	3.5	12
39	Prediction of Acute Aquatic Toxicity toward Daphnia Magna by using the GA-kNN Method. ATLA Alternatives To Laboratory Animals, 2014, 42, 31-41.	1.0	59
40	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
41	Towards Global QSAR Model Building for Acute Toxicity: Munro Database Case Study. International Journal of Molecular Sciences, 2014, 15, 18162-18174.	4.1	36
42	QSPR STUDY OF RHEOLOGICAL AND MECHANICAL PROPERTIES OF CHLOROPRENE RUBBER ACCELERATORS. Rubber Chemistry and Technology, 2014, 87, 219-238.	1.2	7
43	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
44	Reshaped Sequential Replacement algorithm: An efficient approach to variable selection. Chemometrics and Intelligent Laboratory Systems, 2014, 133, 136-148.	3.5	17
45	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	6.4	1,401
46	K-CM: A new artificial neural network. Application to supervised pattern recognition. Chemometrics and Intelligent Laboratory Systems, 2014, 138, 110-119.	3.5	20
47	A novel variable reduction method adapted from space-filling designs. Chemometrics and Intelligent Laboratory Systems, 2014, 136, 147-154.	3.5	60
48	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
49	Locally centred Mahalanobis distance: A new distance measure with salient features towards outlier detection. Analytica Chimica Acta, 2013, 787, 1-9.	5.4	60
50	Quantitative Structureâ€“Activity Relationship Models for Ready Biodegradability of Chemicals. Journal of Chemical Information and Modeling, 2013, 53, 867-878.	5.4	160
51	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
52	Comparison of Different Approaches to Define the Applicability Domain of QSAR Models. Molecules, 2012, 17, 4791-4810.	3.8	370
53	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
54	Assessing bioaccumulation of polybrominated diphenyl ethers for aquatic species by QSAR modeling. Chemosphere, 2012, 89, 433-444.	8.2	28

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55	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
56	Sensitivity assessment of freshwater macroinvertebrates to pesticides using biological traits. Ecotoxicology, 2012, 21, 336-352.	2.4	37
57	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
58	The j-index: a new bibliometric index and multivariate comparisons between other common indices. Scientometrics, 2011, 87, 621-639.	3.0	29
59	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
60	Structure â€“Activity Relationships by Autocorrelation Descriptors and Genetic Algorithms. , 2011, , 60-94.		4
61	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
62	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
63	Evaluation of model predictive ability by external validation techniques. Journal of Chemometrics, 2010, 24, 194-201.	1.3	290
64	Geographical Characterization of Olive Oil by Means of Multivariate Classification. , 2010, , 129-137.		0
65	Self Organizing Maps for Analysis of Polycyclic Aromatic Hydrocarbons 3-Way Data from Spilled Oils. Analytical Chemistry, 2010, 82, 4264-4271.	6.5	13
66	Molecular Descriptors. Challenges and Advances in Computational Chemistry and Physics, 2010, , 29-102.	0.6	62
67	Multicriteria Decision-Making Methods. , 2009, , 585-615.		3
68	Dairy cream response in instrumental texture evaluation processed by multivariate analysis. Chemometrics and Intelligent Laboratory Systems, 2009, 96, 258-263.	3.5	3
69	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
70	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
71	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
72	Comments on the Definition of the Q² Parameter for QSAR Validation. Journal of Chemical Information and Modeling, 2009, 49, 1669-1678.	5.4	483

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73	Multivariate Classification for Qualitative Analysis. , 2009, , 83-104.		50
74	Multicriteria Decision-Making Methods. , 2009, , 591-629.		29
75	Chemometrics in QSAR. , 2009, , 129-172.		38
76	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
77	Chapter 2 Total-Order Ranking Methods. Data Handling in Science and Technology, 2008, 27, 51-72.	3.1	9
78	Chapter 9 The DART (Decision Analysis by Ranking Techniques) Software. Data Handling in Science and Technology, 2008, , 193-207.	3.1	6
79	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
80	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
81	Classification of multiway analytical data based on MOLMAP approach. Analytica Chimica Acta, 2007, 605, 134-146.	5.4	17
82	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
83	New QSAR Modelling Approach Based on Ranking Models by Genetic Algorithms - Variable Subset Selection (GA-VSS). , 2006, , 181-217.		8
84	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
85	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
86	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
87	Virtual Computational Chemistry Laboratory â€“ Design and Description. Journal of Computer-Aided Molecular Design, 2005, 19, 453-463.	2.9	1,250
88	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
89	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
90	New indices for analysing partial ranking diagrams. Analytica Chimica Acta, 2004, 515, 167-181.	5.4	30

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91	Detecting â€œbadâ€•regression models: multicriteria fitness functions in regression analysis. Analytica Chimica Acta, 2004, 515, 199-208.	5.4	156
92	Study on anaerobic and aerobic degradation of different non-ionic surfactants. Bioresource Technology, 2003, 87, 87-91.	9.6	25
93	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
94	MobyDigs: software for regression and classification models by genetic algorithms. Data Handling in Science and Technology, 2003, 23, 141-167.	3.1	34
95	The BEAM-project: prediction and assessment of mixture toxicities in the aquatic environment. Continental Shelf Research, 2003, 23, 1757-1769.	1.8	111
96	New 3D Molecular Descriptors: The WHIM theory and QSAR Applications. , 2002, , 355-380.		28
97	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
98	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
99	Steric Control of Conductivity in Highly Conjugated Polythiophenes. Chemistry of Materials, 2001, 13, 1665-1673.	6.7	33
100	QSAR and Chemometric Approaches for Setting Water Quality Objectives for Dangerous Chemicals. Ecotoxicology and Environmental Safety, 2001, 49, 206-220.	6.0	42
101	QSAR approach for the selection of congeneric compounds with a similar toxicological mode of action. Chemosphere, 2001, 42, 873-883.	8.2	41
102	Traditional versus WHIM molecular descriptors in QSAR approaches applied to fish toxicity studies. Chemosphere, 2001, 44, 401-406.	8.2	27
103	A combined use of global and local approaches in 3D-QSAR. Chemometrics and Intelligent Laboratory Systems, 2000, 52, 183-194.	3.5	8
104	Chemometrics for Sampling and Analysis: Theory and Environmental Applications. , 2000, , 387-404.		1
105	A New Molecular Structure Representation: Spectral Weighted Molecular (SWM) Signals and Spectral Weighted Invariant Molecular (SWIM) Descriptors. , 2000, , 344-344.		0
106	QSAR Approach for the Selection of Congeneric Compounds with Similar Toxicological Modes of Action. , 2000, , 292-292.		0
107	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
108	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

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109	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
110	The K correlation index: theory development and its application in chemometrics. Chemometrics and Intelligent Laboratory Systems, 1999, 46, 13-29.	3.5	172
111	QSAR study on the tropospheric degradation of organic compounds. Chemosphere, 1999, 38, 1371-1378.	8.2	67
112	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
113	New 3D molecular descriptors: the WHIM theory and QSAR applications. Journal of Computer - Aided Molecular Design, 1998, 9/11, 355-380.	1.0	71
114	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
115	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
116	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
117	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
118	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
119	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
120	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
121	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
122	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
123	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
124	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
125	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
126	Modeling and prediction by using WHIM descriptors in QSAR studies: submitochondrial particles (SMP) as toxicity blosensors of chlorophenols. Chemosphere, 1996, 33, 71-79.	8.2	41

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127	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
128	Submitochondrial particles as toxicity biosensors of chlorophenols. Environmental Toxicology and Chemistry, 1995, 14, 363-368.	4.3	38
129	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
130	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
131	Steric effects in polybitniophenes. , 1994, , .		0
132	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
133	New molecular descriptors for 2D and 3D structures. Theory. Journal of Chemometrics, 1994, 8, 263-272.	1.3	269
134	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
135	Linear discriminant hierarchical clustering: A modeling and cross-validable divisive clustering method. Chemometrics and Intelligent Laboratory Systems, 1993, 19, 43-51.	3.5	9
136	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
137	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
138	The chemical meaning of topological indices. Chemometrics and Intelligent Laboratory Systems, 1992, 15, 51-59.	3.5	35
139	Linear discriminant classification tree: A user-driven multicriteria classification method. Chemometrics and Intelligent Laboratory Systems, 1992, 16, 25-35.	3.5	15
140	A new algorithm for optimal, distance-based experimental design. Chemometrics and Intelligent Laboratory Systems, 1992, 16, 37-44.	3.5	99
141	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
142	A chemometric approach for evaluating the efficiency of a pilot plant for MSW combustion. Chemosphere, 1991, 23, 1407-1416.	8.2	4
143	A fast method for the calculation of partial least squares coefficients. Chemometrics and Intelligent Laboratory Systems, 1991, 12, 117-120.	3.5	15
144	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

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145	Methodologies for the identification of the pharmacophore in series of bioactive compounds. Journal of Molecular Graphics, 1991, 9, 70.	1.1	2
146	Rabbit nest construction and its relationship with litter development. Applied Animal Behaviour Science, 1991, 31, 259-266.	1.9	29
147	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
148	Pharmacophore Identification in Amnesia-Reversal Compounds Using Conformational Analysis and Chemometric Methods. QSAR and Combinatorial Science, 1990, 9, 195-201.	1.2	15
149	Weighted k-Nearest Neighbour Method for the Calculation of Missing Values. Chemometrics and Intelligent Laboratory Systems, 1990, 9, 201-205.	3.5	11
150	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
151	k-nearest neighbour method: The influence of data transformations and metrics. Chemometrics and Intelligent Laboratory Systems, 1989, 6, 213-220.	3.5	25
152	School of Chemometrics, Cuenca, Ecuador, 8â€“12 May 1989. Chemometrics and Intelligent Laboratory Systems, 1989, 6, 258.	3.5	0
153	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
154	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
155	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
156	PCDD and PCDF in emissions from the combustion of MSW in a pilot plant. Preliminary results. Chemosphere, 1989, 19, 417-422.	8.2	9
157	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
158	Theoretical studies of stereoselective aldol condensations. Journal of Organic Chemistry, 1986, 51, 612-616.	3.2	36
159	Lewis acid mediated aldol condensations using thioester silyl ketene acetals. Tetrahedron, 1986, 42, 893-909.	1.9	87
160	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
161	Stereoselective aldol condensations via alkenyloxy dialkoxyboranes : mechanistic and stereochemical details. Tetrahedron, 1984, 40, 4051-4058.	1.9	27
162	Conformational studies of octalene and its benzo-derivatives. Journal of Computational Chemistry, 1984, 5, 343-348.	3.3	1

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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	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
165	Conformation of bicyclo [n.1.0] derivatives. Computational and Theoretical Chemistry, 1983, 105, 17-29.	1.5	2
166	The conformation of 1-vinylcyclohexene. Computational and Theoretical Chemistry, 1983, 105, 291-306.	1.5	1
167	CONFORMATIONAL ANALYSIS OF TRIMETHYLPHOSPHITE AND ITS METAL COMPLEXES. Phosphorous and Sulfur and the Related Elements, 1983, 17, 205-220.	0.2	9
168	Conformation of bicyclo [n.1.0] Derivatives. Computational and Theoretical Chemistry, 1982, 87, 53-64.	1.5	11
169	Conformation of bicyclo [n.1.0] derivatives. Computational and Theoretical Chemistry, 1982, 90, 165-176.	1.5	3
170	Geometry and energy of overcrowded ethylenes. II. Bornanylidene, fenchylidene, and bifluorenylidene derivatives. Journal of Computational Chemistry, 1982, 3, 178-184.	3.3	18
171	Conformation of bicyclo[n.1.0] derivatives. Journal of Molecular Structure, 1982, 90, 165-176.	3.6	4
172	Conformational analysis of polysubstituted ethanes. Journal of the American Chemical Society, 1981, 103, 3679-3682.	13.7	12
173	Electro-optical properties of the oxirane skeleton and the carbonâ€“carbon bond in its derivatives. Journal of the Chemical Society Faraday Transactions I, 1981, 77, 1611.	1.0	1
174	Geometry and energy of tetra-tert-butylethylene. Journal of Computational Chemistry, 1981, 2, 149-156.	3.3	15
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