Svante Wold

List of Publications by Year
in descending order

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167 papers	36,918 citations	17440 63 h-index	6836 155 g-index
174 all docs	174 docs citations	174 times ranked	30277 citing authors

#	Article	IF	Citations
1	PLS-regression: a basic tool of chemometrics. Chemometrics and Intelligent Laboratory Systems, 2001, 58, 109-130.	3.5	7,224
2	Cross-Validatory Estimation of the Number of Components in Factor and Principal Components Models. Technometrics, 1978, 20, 397-405.	1.9	2,161
3	Orthogonal projections to latent structures (Oâ€PLS). Journal of Chemometrics, 2002, 16, 119-128.	1.3	1,958
4	Pattern recognition by means of disjoint principal components models. Pattern Recognition, 1976, 8, 127-139.	8.1	1,040
5	Orthogonal signal correction of near-infrared spectra. Chemometrics and Intelligent Laboratory Systems, 1998, 44, 175-185.	3.5	911
6	Multi-way principal components-and PLS-analysis. Journal of Chemometrics, 1987, 1, 41-56.	1.3	670
7	CVâ€ANOVA for significance testing of PLS and OPLSÂ® models. Journal of Chemometrics, 2008, 22, 594-600.	1.3	600
8	Cross-Validatory Estimation of the Number of Components in Factor and Principal Components Models. Technometrics, 1978, 20, 397.	1.9	586
9	New Chemical Descriptors Relevant for the Design of Biologically Active Peptides. A Multivariate Characterization of 87 Amino Acids. Journal of Medicinal Chemistry, 1998, 41, 2481-2491.	6.4	574
10	Peptide quantitative structure-activity relationships, a multivariate approach. Journal of Medicinal Chemistry, 1987, 30, 1126-1135.	6.4	509
11	Nonlinear PLS modeling. Chemometrics and Intelligent Laboratory Systems, 1989, 7, 53-65.	3.5	478
12	Some recent developments in PLS modeling. Chemometrics and Intelligent Laboratory Systems, 2001, 58, 131-150.	3.5	442
13	Partial least-squares method for spectrofluorimetric analysis of mixtures of humic acid and lignin sulfonate. Analytical Chemistry, 1983, 55, 643-648.	6.5	440
14	Partial least squares analysis with cross-validation for the two-class problem: A Monte Carlo study. Journal of Chemometrics, 1987, 1, 185-196.	1.3	435
15	SIMCA: A Method for Analyzing Chemical Data in Terms of Similarity and Analogy. ACS Symposium Series, 1977, , 243-282.	0.5	363
16	Modelling and diagnostics of batch processes and analogous kinetic experiments. Chemometrics and Intelligent Laboratory Systems, 1998, 44, 331-340.	3.5	332
17	Spline Functions in Data Analysis. Technometrics, 1974, 16, 1-11.	1.9	307
18	O2-PLS, a two-block (X-Y) latent variable regression (LVR) method with an integral OSC filter. Journal of Chemometrics, 2003, 17, 53-64.	1.3	301

#	Article	IF	Citations
19	Multivariate Data Analysis in Chemistry. , 1984, , 17-95.		300
20	Hierarchical multiblock PLS and PC models for easier model interpretation and as an alternative to variable selection. Journal of Chemometrics, 1996, 10, 463-482.	1.3	294
21	The kernel algorithm for PLS. Journal of Chemometrics, 1993, 7, 45-59.	1.3	292
22	A PLS kernel algorithm for data sets with many variables and fewer objects. Part 1: Theory and algorithm. Journal of Chemometrics, 1994, 8, 111-125.	1.3	270
23	Validation of QSAR's. QSAR and Combinatorial Science, 1991, 10, 191-193.	1.2	266
24	An evaluation of orthogonal signal correction applied to calibration transfer of near infrared spectra. Chemometrics and Intelligent Laboratory Systems, 1998, 44, 229-244.	3.5	256
25	Nonlinear partial least squares modelling II. Spline inner relation. Chemometrics and Intelligent Laboratory Systems, 1992, 14, 71-84.	3.5	249
26	Using chemometrics for navigating in the large data sets of genomics, proteomics, and metabonomics (gpm). Analytical and Bioanalytical Chemistry, 2004, 380, 419-429.	3.7	245
27	A multivariate calibration problem in analytical chemistry solved by partial least-squares models in latent variables. Analytica Chimica Acta, 1983, 150, 61-70.	5.4	242
28	Exponentially weighted moving principal components analysis and projections to latent structures. Chemometrics and Intelligent Laboratory Systems, 1994, 23, 149-161.	3.5	226
29	Interactive variable selection (IVS) for PLS. Part 1: Theory and algorithms. Journal of Chemometrics, 1994, 8, 349-363.	1.3	210
30	Adaptive batch monitoring using hierarchical PCA. Chemometrics and Intelligent Laboratory Systems, 1998, 41, 73-81.	3.5	171
31	Four levels of pattern recognition. Analytica Chimica Acta, 1978, 103, 429-443.	5.4	166
32	PLS regression on wavelet compressed NIR spectra. Chemometrics and Intelligent Laboratory Systems, 1998, 42, 209-220.	3.5	165
33	Principal component analysis of multivariate images. Chemometrics and Intelligent Laboratory Systems, 1989, 5, 209-220.	3.5	160
34	PCA and PLS with very large data sets. Computational Statistics and Data Analysis, 2005, 48, 69-85.	1.2	154
35	Multivariate quantitative structure-activity relationships (QSAR): conditions for their applicability. Journal of Chemical Information and Computer Sciences, 1983, 23, 6-13.	2.8	152
36	Multivariate analysis of aquatic toxicity data with PLS. Aquatic Sciences, 1995, 57, 217-241.	1.5	137

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37	6 Multivariate Data Analysis and Experimental Design in Biomedical Research. Progress in Medicinal Chemistry, 1988, 25, 291-338.	10.4	134
38	Residual bilinearization. Part 1: Theory and algorithms. Journal of Chemometrics, 1990, 4, 79-90.	1.3	130
39	Chemometrics, present and future success. Chemometrics and Intelligent Laboratory Systems, 1998, 44, 3-14.	3.5	125
40	Minimum analogue peptide sets (MAPS) for quantitative structureâ€activity relationships. International Journal of Peptide and Protein Research, 1991, 37, 414-424.	0.1	124
41	A randomization test for PLS component selection. Journal of Chemometrics, 2007, 21, 427-439.	1.3	122
42	The Prediction of Bradykinin Potentiating Potency of Pentapeptides. An Example of a Peptide Quantitative Structure-activity Relationship.. Acta Chemica Scandinavica, 1986, 40b, 135-140.	0.7	112
43	Multivariate design. Analytica Chimica Acta, 1986, 191, 17-32.	5.4	111
44	Multivariate Parametrization of 55 Coded and Non-Coded Amino Acids. QSAR and Combinatorial Science, 1989, 8, 204-209.	1.2	107
45	INLR, implicit non-linear latent variable regression. Journal of Chemometrics, 1997, 11, 141-156.	1.3	102
46	A multivariate study of the relationship between the genetic code and the physical-chemical properties of amino acids. Journal of Molecular Evolution, 1985, 22, 272-277.	1.8	98
47	Source contributions to ambient aerosol calculated by discriminat partial least squares regression (PLS). Journal of Chemometrics, 1988, 2, 281-296.	1.3	91
48	Screening of Suitable Solvents in Organic Synthesis. Strategies for Solvent Selection.. Acta Chemica Scandinavica, 1985, 39b, 79-91.	0.7	91
49	On the selection of the training set in environmental QSAR analysis when compounds are clustered. Journal of Chemometrics, 2000, 14, 599-616.	1.3	88
50	Statistical Molecular Design of Building Blocks for Combinatorial Chemistry. Journal of Medicinal Chemistry, 2000, 43, 1320-1328.	6.4	86
51	Personal memories of the early PLS development. Chemometrics and Intelligent Laboratory Systems, 2001, 58, 83-84.	3.5	86
52	PLS DISCRIMINANT PLOTS. , 1986, , 461-470.		85
53	Orthogonal signal correction, wavelet analysis, and multivariate calibration of complicated process fluorescence data. Analytica Chimica Acta, 2000, 420, 181-195.	5.4	83
54	Multivariate analysis of variance (MANOVA). Chemometrics and Intelligent Laboratory Systems, 1990, 9, 127-141.	3.5	82

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55	Evaluation of a multiple gas mixture with a simple MOSFET gas sensor array and pattern recognition. Sensors and Actuators B: Chemical, 1990, 2, 115-123.	7.8	75
56	Interactive variable selection (IVS) for PLS. Part II: Chemical applications. Journal of Chemometrics, 1995, 9, 331-342.	1.3	74
57	Principal property values for six non-natural amino acids and their application to a structureâ€“activity relationship for oxytocin peptide analogues. Canadian Journal of Chemistry, 1987, 65, 1814-1820.	1.1	73
58	Classification of fungi by means of pyrolysis-gas chromatography-pattern recognition. Journal of Chromatography A, 1979, 173, 19-32.	3.7	69
59	D-optimal onion designs in statistical molecular design. Chemometrics and Intelligent Laboratory Systems, 2004, 73, 37-46.	3.5	69
60	Major components influencing retention indices in gas chromatography. Journal of Chromatography A, 1973, 80, 43-59.	3.7	68
61	D-Optimal Designs in QSAR. QSAR and Combinatorial Science, 1993, 12, 225-231.	1.2	68
62	Multivariate process and quality monitoring applied to an electrolysis process. Chemometrics and Intelligent Laboratory Systems, 1998, 42, 221-231.	3.5	67
63	Structure-activity study of .beta.-adrenergic agents using the SIMCA method of pattern recognition. Journal of Medicinal Chemistry, 1978, 21, 922-930.	6.4	64
64	Residual bilinearization. Part 2: Application to HPLCâ€”diode array data and comparison with rank annihilation factor analysis. Journal of Chemometrics, 1990, 4, 135-146.	1.3	62
65	Structure-activity analyzed by pattern recognition: the asymmetric case. Journal of Medicinal Chemistry, 1980, 23, 595-599.	6.4	60
66	Quantitative sequence-activity models (QSAM)â€”tools for sequence design. Nucleic Acids Research, 1993, 21, 733-739.	14.5	58
67	Discussion: PLS in Chemical Practice. Technometrics, 1993, 35, 136-139.	1.9	54
68	A PLS kernel algorithm for data sets with many variables and few objects. Part II: Cross-validation, missing data and examples. Journal of Chemometrics, 1995, 9, 459-470.	1.3	53
69	A structure-carcinogenicity study of 4-nitroquinoline 1-oxides using the SIMCA method of pattern recognition. Journal of Medicinal Chemistry, 1978, 21, 1001-1007.	6.4	51
70	Local principal component models, rank maps and contextuality for curve resolution and multi-way calibration inference. Chemometrics and Intelligent Laboratory Systems, 1987, 2, 273-281.	3.5	50
71	Statistical Molecular Design, Parallel Synthesis, and Biological Evaluation of a Library of Thrombin Inhibitors. Journal of Medicinal Chemistry, 2001, 44, 3424-3439.	6.4	50
72	A chemometrics toolbox based on projections and latent variables. Journal of Chemometrics, 2014, 28, 332-346.	1.3	50

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73	Megavariate analysis of hierarchical QSAR data. Journal of Computer-Aided Molecular Design, 2002, 16, 711-726.	2.9	49
74	Relationships between chemical structure and biological activity modeled by SIMCA pattern recognition. Bioorganic Chemistry, 1980, 9, 505-523.	4.1	48
75	Image analysis and chemical information in images. Analytica Chimica Acta, 1986, 191, 473-480.	5.4	48
76	Comments on a recent evaluation of the SIMCA method. Journal of Chemometrics, 1987, 1, 243-245.	1.3	47
77	A strategy for ranking environmentally occurring chemicals. Chemometrics and Intelligent Laboratory Systems, 1989, 5, 169-186.	3.5	47
78	A serial extension of multiblock PLS. Journal of Chemometrics, 1999, 13, 461-471.	1.3	47
79	Calibration Transfer for Predicting Lake-Water pH from near Infrared Spectra of Lake Sediments. Journal of Near Infrared Spectroscopy, 1999, 7, 251-264.	1.5	44
80	Data analysis of pyrolysisâ€"chromatograms by means of simca pattern recognition. Journal of Analytical and Applied Pyrolysis, 1979, 1, 53-65.	5.5	43
81	31 Pattern recognition in chemistry. Handbook of Statistics, 1982, 2, 673-697.	0.6	43
82	Chemometrics, why, what and where to next?. Journal of Pharmaceutical and Biomedical Analysis, 1991, 9, 589-596.	2.8	43
83	Carcinogenicity of Polycyclic Aromatic Hydrocarbons Studied by SIMCA Pattern Recognition.. Acta Chemica Scandinavica, 1978, 32b, 602-608.	0.7	42
84	The Anesthetic Activity and Toxicity of Halogenated Ethyl Methyl Ethers, a Multivariate QSAR Modelled by PLS. QSAR and Combinatorial Science, 1985, 4, 1-11.	1.2	39
85	Multivariate resolution of overlapped peaks in liquid chromatography using diode array detection. Analytical Chemistry, 1986, 58, 299-303.	6.5	38
86	New and old trends in chemometrics. How to deal with the increasing data volumes in R&D&P (research, development and production)?with examples from pharmaceutical research and process modeling. Journal of Chemometrics, 2002, 16, 377-386.	1.3	37
87	On the use of some multivariate statistical methods in pharmacological research. Journal of Pharmacological Methods, 1986, 16, 91-110.	0.7	36
88	The utility of multivariate design in PLS modeling. Journal of Chemometrics, 2004, 18, 156-165.	1.3	36
89	Application of simca multivariate data analysis to the classification of gas chromatographic profiles of human brain tissues. Analytica Chimica Acta, 1981, 133, 251-259.	5.4	35
90	A STRATEGY FOR RANKING ENVIRONMENTALLY OCCURRING CHEMICALS. PART III: MULTIVARIATE QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIPS FOR HALOGENATED ALIPHATICS. Environmental Toxicology and Chemistry, 1990, 9, 1339.	4.3	35

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91	Plasma Levels and Clinical Effects of Thioridazine and Thiothixene. Journal of Clinical Pharmacology, 1975, 15, 178-186.	2.0	34
92	Distribution of arsenic, manganese, and selenium in the human brain in chronic renal insufficiency, Parkinson's disease, and amyotrophic lateral sclerosis. Journal of the Neurological Sciences, 1981, 51, 437-446.	0.6	33
93	Preference of cauliflower related to sensory descriptive variables by partial least squares (PLS) regression. Journal of the Science of Food and Agriculture, 1983, 34, 715-724.	3.5	33
94	QSARs based on statistical design and their use for identifying chemicals for further biological testing. Environmental Toxicology and Chemistry, 1990, 9, 265-277.	4.3	33
95	Kernel-based PLS regression; Cross-validation and applications to spectral data. Journal of Chemometrics, 1994, 8, 377-389.	1.3	31
96	Study of Preprocessing Methods for the Determination of Crystalline Phases in Binary Mixtures of Drug Substances by X-ray Powder Diffraction and Multivariate Calibration. Applied Spectroscopy, 2000, 54, 1222-1230.	2.2	30
97	The GIFI approach to non-linear PLS modeling. Journal of Chemometrics, 2001, 15, 321-336.	1.3	29
98	Reproducibility of pyrolysis-gas chromatographic analyses of the mould penicillim brevi-compactum. Journal of Chromatography A, 1979, 173, 7-17.	3.7	28
99	Comparison Between X-Ray Crystallographic Data and Physicochemical Parameters with Respect to Their Information about the Calcium Channel Antagonist Activity of 4-Phenyl-1,4-dihydropyridines. QSAR and Combinatorial Science, 1986, 5, 45-50.	1.2	28
100	Multivariate process and quality monitoring applied to an electrolysis process. Chemometrics and Intelligent Laboratory Systems, 1998, 42, 233-240.	3.5	28
101	Chemometrics and its Roots in Physical Organic Chemistry.. Acta Chemica Scandinavica, 1998, 52, 517-523.	0.7	28
102	Analogy Models for Prediction of Human Toxicity. ATLA Alternatives To Laboratory Animals, 1990, 18, 103-116.	1.0	28
103	Cluster-based Design in Environmental QSAR. QSAR and Combinatorial Science, 1997, 16, 383-390.	1.2	27
104	Multivariate design of process experiments (M-DOPE). Chemometrics and Intelligent Laboratory Systems, 1994, 23, 39-50.	3.5	26
105	Fuzzy clustering of 627 alcohols, guided by a strategy for cluster analysis of chemical compounds for combinatorial chemistry. Chemometrics and Intelligent Laboratory Systems, 1998, 44, 213-227.	3.5	26
106	Multivariate Parametrization of Amino Acid Properties by Thin Layer Chromatography. QSAR and Combinatorial Science, 1988, 7, 144-150.	1.2	25
107	Relationships between higher-order data array configurations and problem formulations in multivariate data analysis. Journal of Chemometrics, 1989, 3, 33-48.	1.3	23
108	Statistical molecular design of peptoid libraries. Molecular Diversity, 1998, 4, 103-114.	3.9	23

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109	A strategy for ranking environmentally occurring chemicals. Chemometrics and Intelligent Laboratory Systems, 1989, 7, 131-141.	3.5	20
110	Sampling Reproducibility and Error Estimation in near Infrared Calibration of Lake Sediments for Water Quality Monitoring. Journal of Near Infrared Spectroscopy, 1999, 7, 241-250.	1.5	20
111	Multivariate quantitative structure-activity relationships for the aquatic toxicity of technical nonionic surfactants. Journal of Surfactants and Detergents, 2000, 3, 33-41.	2.1	20
112	Peptide QSAR on Substance P Analogues, Enkephalins, and Bradykinins Containing L- and D-Amino Acids.. Acta Chemica Scandinavica, 1990, 44, 50-55.	0.7	20
113	Time-resolved QSAR: an approach to PLS modelling of three-way biological data. Chemometrics and Intelligent Laboratory Systems, 2004, 73, 73-84.	3.5	19
114	Interpretation of NMR substituent parameters by the use of a pattern recognition approach. Journal of Magnetic Resonance, 1980, 37, 183-194.	0.5	18
115	Application of principal component analysis to13C NMR shifts of chalcones and their thiophene and furan analogues: A useful tool for the shift assignment and for the study of substituent effects. Magnetic Resonance in Chemistry, 1981, 17, 118-123.	0.7	18
116	Principal components and partial least-squares analysis of the geochemistry of volcanic rocks from the aeolian archipelago. Analytica Chimica Acta, 1983, 150, 129-143.	5.4	18
117	Simultaneous determination of five different food proteins by high-performance liquid chromatography and partial least-squares multivariate calibration. Analytica Chimica Acta, 1985, 174, 41-51.	5.4	18
118	Alignment of flexible molecules at their receptor site using 3D descriptors and Hi-PCA. Journal of Computer-Aided Molecular Design, 1997, 11, 601-612.	2.9	18
119	Comparison between physicochemical and calculated molecular descriptors. Journal of Chemometrics, 2000, 14, 629-642.	1.3	18
120	PLSâ€treesÂ®, a topâ€down clustering approach. Journal of Chemometrics, 2009, 23, 569-580.	1.3	17
121	Discussion: PLS in Chemical Practice. Technometrics, 1993, 35, 136.	1.9	17
122	GIFI-PLS: Modeling of Non-Linearities and Discontinuities in QSAR. QSAR and Combinatorial Science, 2000, 19, 345-355.	1.2	16
123	Multivariate analysis of congruent images (MACI). Journal of Chemometrics, 2005, 19, 393-403.	1.3	16
124	Linear Free Energy Relationships as Tools for Investigating Chemical Similarityâ€"Theory and Practice. , 1978, , 1-54.		15
125	The carcinogenicity of N-nitroso compounds: A SIMCA pattern recognition study. Bioorganic Chemistry, 1981, 10, 29-45.	4.1	15
126	Simplified C-13 NMR Parameters Related to the Carcinogenic Potency of Polycyclic Aromatic Hydrocarbons. QSAR and Combinatorial Science, 1983, 2, 73-76.	1.2	15

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127	QSAR Modelling of the Toxicity of some Technical Non-ionic Surfactants towards Fairy Shrimps. QSAR and Combinatorial Science, 1996, 15, 208-218.	1.2	15
128	Controlling coverage of D-optimal onion designs and selections. Journal of Chemometrics, 2004, 18, 548-557.	1.3	15
129	Determination of the proteins in mixtures of meat, soymeal and rind from their chromatographic amino-acid pattern by the partial least-squares method. Analytica Chimica Acta, 1985, 171, 1-11.	5.4	14
130	Relationships between induction of anesthesia and mitotic spindle disturbances studied by means of principal component analysis. Mutation Research-Fundamental and Molecular Mechanisms of Mutagenesis, 1986, 174, 109-113.	1.1	14
131	Separating Y-predictive and Y-orthogonal variation in multi-block spectral data. Journal of Chemometrics, 2006, 20, 352-361.	1.3	14
132	A Multivariate Representation and Analysis of DNA Sequence Data.. Acta Chemica Scandinavica, 1991, 45, 186-192.	0.7	14
133	Multivariate Characterization of Amino Acids by Reversed Phase High Pressure Liquid Chromatography. QSAR and Combinatorial Science, 1987, 6, 158-164.	1.2	13
134	Strategies for subset selection of parts of an in-house chemical library. Journal of Chemometrics, 2001, 15, 353-369.	1.3	13
135	Multivariate modelling of geochemical and geophysical exploration data. Chemometrics and Intelligent Laboratory Systems, 1987, 2, 161-175.	3.5	12
136	A strategy for ranking environmentally occurring chemicals. Part V: The development of two genotoxicity QSARs for halogenated aliphatics. Environmental Toxicology and Chemistry, 1991, 10, 585-596.	4.3	12
137	Quantitative-structure-effect relationship for some technical nonionic surfactants. JAOCS, Journal of the American Oil Chemists' Society, 1996, 73, 863-875.	1.9	12
138	Modelling the Cytotoxicity of Halogenated Aliphatic Hydrocarbons. Quantitative Structure-Activity Relationships for the IC50to Human HeLa Cells. QSAR and Combinatorial Science, 1993, 12, 124-131.	1.2	11
139	A Strategy for Ranking Environmentally Occurring Chemicals. Part IV: Development of Chemical Model Systems for Characterization of Halogenated Aliphatic Hydrocarbons. QSAR and Combinatorial Science, 1991, 10, 36-42.	1.2	10
140	Intelligent Combinatorial Libraries. , 0, , 189-208.		10
141	Multivariate geochemical modelling and integration with petrophysical data. Journal of Geochemical Exploration, 1987, 29, 279-294.	3.2	9
142	Dedicated principal properties for peptide QSARs: Theory and applications. Journal of Chemometrics, 1990, 4, 241-253.	1.3	9
143	A strategy for ranking environmentally occurring chemicals. Part III: Multivariate quantitative structure-activity relationships for halogenated aliphatics. Environmental Toxicology and Chemistry, 2010, 9, 1339-1351.	4.3	9
144	Trace-element concentrations in blood samples from welders of stainless steel or aluminium and a reference group.. Scandinavian Journal of Work, Environment and Health, 1977, 3, 183-191.	3.4	9

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145	Temperature dependence of the heat capacity of activation (.DELTA.Cp.ddg.) for solvolysis reactions in water. The Journal of Physical Chemistry, 1972, 76, 369-374.	2.9	8
146	A Strategy for Ranking Environmentally Occurring Chemicals. Part VI. QSARs for the Mutagenic Effects of Halogenated Aliphatics.. Acta Chemica Scandinavica, 1991, 45, 935-944.	0.7	8
147	A Simca Pattern Recognition Study in Taxonomy: Claw Shape in Mosquitoes (Culicidae, Insecta). Systematic Zoology, 1984, 33, 355.	1.6	6
148	PLS modelling of detergency performance for some technical nonionic surfactants. Chemometrics and Intelligent Laboratory Systems, 1996, 32, 111-124.	3.5	6
149	A graphical index of separation (GIOS) in multivariate modeling. Journal of Chemometrics, 2010, 24, 779-789.	1.3	6
150	Estimation of Activation Parameters from One Kinetic Experiment (Varytemp Method). Error Analysis and Revised Computer Program.. Acta Chemica Scandinavica, 1971, 25, 336-339.	0.7	6
151	Rational ranking of chemicals according to environmental risk. Chemometrics and Intelligent Laboratory Systems, 1992, 14, 245-252.	3.5	5
152	CHARACTERIZATION AND CLASSIFICATION BASED ON MULTIVARIATE DATA ANALYSIS. , 1980, , 377-386.		5
153	Pattern-recognition Search for the Basic Regularities in the Stability of Complex Hydrides. Part 1. A Simplified Model.. Acta Chemica Scandinavica, 1977, 31a, 391-401.	0.7	5
154	Use of chemometrics in environmental toxicology and structure-activity relationships. TrAC - Trends in Analytical Chemistry, 1986, 5, 53-56.	11.4	4
155	Multivariate Design and Modelling in QSAR, Combinatorial Chemistry, and Bioinformatics. , 2000, , 27-45.		4
156	Pls and NIR Spectroscopyâ€"Some Recent Developments. NIR News, 1998, 9, 10-11.	0.3	2
157	The Constrained Principal Property (CPP) Space in QSAR â€" Directional and Non-Directional Modelling Approaches. , 2000, , 65-70.		2
158	Society, Politics, and Economic Development Revisited. , 1980, , 1-18.		2
159	Design of Small Libraries for Lead Exploration. , 2002, , 197-220.		2
160	Simple Modeling by Chemical Analogy Pattern Recognition. ACS Symposium Series, 1985, , 243-249.	0.5	1
161	The evolutionary transition from uracil to thymine balances the genetic code. Journal of Chemometrics, 1996, 10, 163-170.	1.3	1
162	INLR (Implicit Non-linear Latent variable Regression). II. Blockscaling of Expanded Terms with QSAR Examples. , 0, , 65-79.		1

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163	The use of Simca Pattern Recognition in the Analysis of Complex Chromatographic Data. , 1984, , 75-88.		1
164	Stone and jonathan versus mager debate. Journal of Chemometrics, 1995, 9, 230-231.	1.3	0
165	Multivariate Techniques for Studying Short Protein Sequences. IFAC Postprint Volumes IPPV / International Federation of Automatic Control, 2001, 34, 69-74.	0.4	0
166	Chemometrics and Bruce: Some Fond Memories. ACS Symposium Series, 2015, , 1-13.	0.5	0
167	Quantitative description of nucleic acid sequences based on chemical characterization of the monomers. , 1993, , 483-484.		0