Ron Wehrens

List of Publications by Year
in descending order

115 papers	6,476 citations	76196 40 h-index	71532 76 g-index
120 all docs	120 docs citations	120 times ranked	10003 citing authors

#	Article	IF	Citations
1	TheplsPackage: Principal Component and Partial Least Squares Regression inR. Journal of Statistical Software, 2007, 18, .	1.8	1,047
2	Self- and Super-organizing Maps inR: ThekohonenPackage. Journal of Statistical Software, 2007, 21, .	1.8	465
3	The bootstrap: a tutorial. Chemometrics and Intelligent Laboratory Systems, 2000, 54, 35-52.	1.8	399
4	Possibilities of visibleâ€“near-infrared spectroscopy for the assessment of soil contamination in river floodplains. Analytica Chimica Acta, 2001, 446, 97-105.	2.6	202
5	Chemometrics with R. , 2011, , .		187
6	Flexible Self-Organizing Maps in kohonen 3.0. Journal of Statistical Software, 2018, 87, .	1.8	183
7	Supervised Kohonen networks for classification problems. Chemometrics and Intelligent Laboratory Systems, 2006, 83, 99-113.	1.8	174
8	Improved batch correction in untargeted MS-based metabolomics. Metabolomics, 2016, 12, 88.	1.4	167
9	Exploring field vegetation reflectance as an indicator of soil contamination in river floodplains. Environmental Pollution, 2004, 127, 281-290.	3.7	156
10	The potential of field spectroscopy for the assessment of sediment properties in river floodplains. Analytica Chimica Acta, 2003, 484, 189-200.	2.6	129
11	A generalized expression for the similarity of spectra: application to powder diffraction pattern classification. Journal of Computational Chemistry, 2001, 22, 273-289.	1.5	112
12	Tomato Fruit Detection and Counting in Greenhouses Using Deep Learning. Frontiers in Plant Science, 2020, 11, 571299.	1.7	104
13	KNN-kernel density-based clustering for high-dimensional multivariate data. Computational Statistics and Data Analysis, 2006, 51, 513-525.	0.7	99
14	Identification of novel functional TBP-binding sites and general factor repertoires. EMBO Journal, 2007, 26, 944-954.	3.5	97
15	The WEIZMASS spectral library for high-confidence metabolite identification. Nature Communications, 2016, 7, 12423.	5.8	95
16	Flash Chemistry Extensively Optimized: Highâ€Temperature Swernâ€“Moffatt Oxidation in an Automated Microreactor Platform. Chemistry - an Asian Journal, 2010, 5, 799-805.	1.7	83
17	Identification of Novel Regulators Associated With Early-Phase Osteoblast Differentiation. Journal of Bone and Mineral Research, 2004, 19, 947-958.	3.1	82
18	Clustering multispectral images: a tutorial. Chemometrics and Intelligent Laboratory Systems, 2005, 77, 3-17.	1.8	82

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19	Multivariate statistical process control using mixture modelling. Journal of Chemometrics, 2005, 19, 23-31.	0.7	81
20	Evolutionary optimisation: a tutorial. TrAC - Trends in Analytical Chemistry, 1998, 17, 193-203.	5.8	80
21	Direct determination of molecular constants from rovibronic spectra with genetic algorithms. Journal of Chemical Physics, 2000, 113, 7955-7962.	1.2	77
22	Assessment of techniques for DOSY NMR data processing. Analytica Chimica Acta, 2003, 490, 231-251.	2.6	77
23	H, C, N and S stable isotopes and mineral profiles to objectively guarantee the authenticity of grated hard cheeses. Analytica Chimica Acta, 2012, 711, 54-59.	2.6	77
24	metaMS: An open-source pipeline for GCâ€“MS-based untargeted metabolomics. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2014, 966, 109-116.	1.2	76
25	Warping methods for spectroscopic and chromatographic signal alignment: A tutorial. Analytica Chimica Acta, 2013, 781, 14-32.	2.6	75
26	LC-MS based global metabolite profiling of grapes: solvent extraction protocol optimisation. Metabolomics, 2012, 8, 175-185.	1.4	72
27	Interpretation of ANOVA models for microarray data using PCA. Bioinformatics, 2007, 23, 184-190.	1.8	70
28	Bootstrapping principal component regression models. , 1997, 11, 157-171.		68
29	Carbon, hydrogen and oxygen stable isotope ratios of whole wood, cellulose and lignin methoxyl groups of Picea abies as climate proxies. Rapid Communications in Mass Spectrometry, 2013, 27, 265-275.	0.7	68
30	Improved parametric time warping for proteomics. Chemometrics and Intelligent Laboratory Systems, 2010, 104, 65-74.	1.8	65
31	Incremental Model-Based Clustering for Large Datasets With Small Clusters. Journal of Computational and Graphical Statistics, 2005, 14, 529-546.	0.9	57
32	Model-Based Clustering for Image Segmentation and Large Datasets via Sampling. Journal of Classification, 2004, 21, 231-253.	1.2	55
33	Climatic and geographical dependence of the H, C and O stable isotope ratios of Italian wine. Analytica Chimica Acta, 2015, 853, 384-390.	2.6	55
34	The use of IRMS, 1 H NMR and chemical analysis to characterise Italian and imported Tunisian olive oils. Food Chemistry, 2016, 196, 98-105.	4.2	55
35	Improved DOSY NMR data processing by data enhancement and combination of multivariate curve resolution with non-linear least square fitting. Journal of Magnetic Resonance, 2004, 169, 257-269.	1.2	54
36	A comparison of methods to relate grass reflectance to soil metal contamination. International Journal of Remote Sensing, 2003, 24, 4995-5010.	1.3	49

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37	A Procedure for Incorporating Spatial Variability in Ecological Risk Assessment of Dutch River Floodplains. Environmental Management, 2001, 28, 359-373.	1.2	48
38	Stability-based biomarker selection. Analytica Chimica Acta, 2011, 705, 15-23.	2.6	47
39	A targeted metabolomics approach to understand differences in flavonoid biosynthesis in red and yellow raspberries. Plant Physiology and Biochemistry, 2013, 72, 79-86.	2.8	47
40	Wavelength selection with Tabu Search. Journal of Chemometrics, 2003, 17, 427-437.	0.7	44
41	Spatial Variability and Uncertainty in Ecological Risk Assessment:Â A Case Study on the Potential Risk of Cadmium for the Little Owl in a Dutch River Flood Plain. Environmental Science & Technology, 2005, 39, 2177-2187.	4.6	42
42	Detecting the addition of sugar and water to wine. Australian Journal of Grape and Wine Research, 2013, 19, 324-330.	1.0	41
43	Initialization of Markov random field clustering of large remote sensing images. IEEE Transactions on Geoscience and Remote Sensing, 2005, 43, 1912-1919.	2.7	40
44	Traceability along the production chain of Italian tomato products on the basis of stable isotopes and mineral composition. Rapid Communications in Mass Spectrometry, 2011, 25, 899-909.	0.7	40
45	SpaRef: a clustering algorithm for multispectral images. Analytica Chimica Acta, 2003, 490, 303-312.	2.6	39
46	Method for the computational comparison of crystal structures. Acta Crystallographica Section B: Structural Science, 2005, 61, 29-36.	1.8	36
47	Use of Metabolic Profiling To Study Grape Skin Polyphenol Behavior as a Result of Canopy Microclimate Manipulation in a â€˜Pinot noirâ€™ Vineyard. Journal of Agricultural and Food Chemistry, 2013, 61, 8976-8986.	2.4	36
48	Fast parametric time warping of peak lists. Bioinformatics, 2015, 31, 3063-3065.	1.8	33
49	A benchmark spikeâ€in data set for biomarker identification in metabolomics. Journal of Chemometrics, 2012, 26, 16-24.	0.7	32
50	Sequential assignment of 2D-NMR spectra of proteins using genetic algorithms. Journal of Chemical Information and Computer Sciences, 1993, 33, 245-251.	2.8	31
51	Transcriptome analysis during berry development provides insights into co-regulated and altered gene expression between a seeded wine grape variety and its seedless somatic variant. BMC Genomics, 2014, 15, 1030.	1.2	31
52	Metabolite variation in the lettuce gene pool: towards healthier crop varieties and food. Metabolomics, 2018, 14, 146.	1.4	31
53	Linking GC-MS and PTR-TOF-MS fingerprints of food samples. Chemometrics and Intelligent Laboratory Systems, 2012, 118, 301-307.	1.8	30
54	Statistical methods for improving verification of claims of origin for Italian wines based on stable isotope ratios. Analytica Chimica Acta, 2012, 757, 19-25.	2.6	29

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55	MetaDB a Data Processing Workflow in Untargeted MS-Based Metabolomics Experiments. Frontiers in Bioengineering and Biotechnology, 2014, 2, 72.	2.0	29
56	Using genetic algorithms for the construction of phylogenetic trees: application to G-protein coupled receptor sequences. BioSystems, 1999, 49, 31-43.	0.9	28
57	HIPS, a hybrid self-adapting expert system for nuclear magnetic resonance spectrum interpretation using genetic algorithms. Analytica Chimica Acta, 1993, 277, 313-324.	2.6	26
58	Constructing a mass measurement error surface to improve automatic annotations in liquid chromatography/mass spectrometry based metabolomics. Rapid Communications in Mass Spectrometry, 2013, 27, 2425-2431.	0.7	25
59	On the Use of1H and13C 1D NMR Spectra as QSPR Descriptors. Journal of Chemical Information and Modeling, 2006, 46, 487-494.	2.5	23
60	Quality Criteria of Genetic Algorithms for Structure Optimization. Journal of Chemical Information and Computer Sciences, 1998, 38, 151-157.	2.8	22
61	The quality of optimisation by genetic algorithms. Analytica Chimica Acta, 1999, 388, 265-271.	2.6	22
62	Hybrid genetic algorithmâ€“tabu search approach for optimising multilayer optical coatings. Analytica Chimica Acta, 2003, 490, 211-222.	2.6	22
63	Mixture modelling of medical magnetic resonance data. Journal of Chemometrics, 2002, 16, 274-282.	0.7	21
64	Stable isotope ratios of H, C, N and O in Italian citrus juices. Journal of Mass Spectrometry, 2014, 49, 785-791.	0.7	21
65	Selfâ€organizing maps: A versatile tool for the automatic analysis of untargeted imaging datasets. Proteomics, 2014, 14, 853-861.	1.3	21
66	High-throughput carotenoid profiling using multivariate curve resolution. Analytical and Bioanalytical Chemistry, 2013, 405, 5075-5086.	1.9	20
67	Multiple comparisons in mass-spectrometry-based -omics technologies. TrAC - Trends in Analytical Chemistry, 2013, 50, 11-21.	5.8	20
68	Molecular data-mining: a challenge for chemometrics. Chemometrics and Intelligent Laboratory Systems, 1999, 49, 121-133.	1.8	18
69	Real-life applications of the MULVADO software package for processing DOSY NMR data. Magnetic Resonance in Chemistry, 2006, 44, 110-117.	1.1	18
70	The Influence of Different Structure Representations on the Clustering of an RNA Nucleotides Data Set. Journal of Chemical Information and Computer Sciences, 2001, 41, 1388-1394.	2.8	16
71	Powder pattern indexing using the weighted crosscorrelation and genetic algorithms. Journal of Computational Chemistry, 2003, 24, 1043-1051.	1.5	15
72	Integrating gene expression and GO classification for PCA by preclustering. BMC Bioinformatics, 2010, 11, 158.	1.2	15

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73	Automatic Phenotyping of Tomatoes in Production Greenhouses Using Robotics and Computer Vision: From Theory to Practice. Agronomy, 2021, 11, 1599.	1.3	15
74	Robust ANOVA for microarray data. Chemometrics and Intelligent Laboratory Systems, 2009, 98, 38-44.	1.8	14
75	F1 hybrid of cultivated apple (MalusÂÃ—Âdomestica) and European pear (Pyrus communis) with fertile F2 offspring. Molecular Breeding, 2014, 34, 817-828.	1.0	14
76	Oxygen and Hydrogen Stable Isotope Ratios of Bulk Needles Reveal the Geographic Origin of Norway Spruce in the European Alps. PLoS ONE, 2015, 10, e0118941.	1.1	14
77	Meta-Statistics for Variable Selection: TheRPackageBioMark. Journal of Statistical Software, 2012, 51, .	1.8	14
78	Circular effects in representations of an RNA nucleotides data set in relation with principal components analysis. Chemometrics and Intelligent Laboratory Systems, 2001, 56, 61-71.	1.8	13
79	Robust DOSY NMR data analysis. Chemometrics and Intelligent Laboratory Systems, 2007, 85, 9-19.	1.8	13
80	Sampling of aquatic sediments. Designs of a decision-support system and a case study. Analytica Chimica Acta, 1993, 271, 11-24.	2.6	12
81	Calibration of an array of voltammetric microelectrodes. Analytica Chimica Acta, 1996, 334, 93-101.	2.6	12
82	Quality criteria of genetic algorithms for construction of phylogenetic trees. , 1999, 20, 867-876.		12
83	Diagnostic analysis of experimental artefacts in DOSY NMR data by covariance matrix of the residuals. Journal of Magnetic Resonance, 2005, 172, 346-358.	1.2	12
84	D-optimal design of an untargeted HS-SPME-GC-TOF metabolite profiling method. Analyst, The, 2012, 137, 3725.	1.7	12
85	A comprehensive full factorial <scp>LC</scp>â€<scp>MS</scp>/<scp>MS</scp> proteomics benchmark data set. Proteomics, 2012, 12, 2276-2281.	1.3	12
86	Metabolite profiling in LCâ€“DAD using multivariate curve resolution: the alsace package for R. Metabolomics, 2015, 11, 143-154.	1.4	12
87	Possibilities of soil spectroscopy for the classification of contaminated areas in river floodplains. International Journal of Applied Earth Observation and Geoinformation, 2001, 3, 337-344.	1.4	11
88	Chemometrics with R. Use R!, 2020, , .	0.3	11
89	Representing structural databases in a self-organizing map. Acta Crystallographica Section B: Structural Science, 2005, 61, 548-557.	1.8	10
90	Thresholding for biomarker selection in multivariate data using Higher Criticism. Molecular BioSystems, 2012, 8, 2339.	2.9	10

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91	LC-MS based plant metabolic profiles of thirteen grassland species grown in diverse neighbourhoods. Scientific Data, 2021, 8, 52.	2.4	10
92	A controlled human intervention trial to study protein quality by amino acid uptake kinetics with the novel Lemna protein concentrate as case study. International Journal of Food Sciences and Nutrition, 2022, 73, 251-262.	1.3	10
93	Supervised Self-Organizing Maps in Crystal Property and Structure Prediction. Crystal Growth and Design, 2007, 7, 1738-1745.	1.4	9
94	Effects of climate change on the distribution of crop wild relatives in the Netherlands in relation to conservation status and ecotope variation. Global Ecology and Conservation, 2020, 23, e01054.	1.0	9
95	Validation and refinement of expert systems: interpretation of NMR spectra as an application in analytical chemistry. Chemometrics and Intelligent Laboratory Systems, 1991, 12, 57-67.	1.8	8
96	Molecular challenges in modern chemometrics. Analytica Chimica Acta, 1999, 400, 413-424.	2.6	8
97	Molecular Chemometrics. Critical Reviews in Analytical Chemistry, 2006, 36, 189-198.	1.8	8
98	Glucosinolate variability between turnip organs during development. PLoS ONE, 2019, 14, e0217862.	1.1	8
99	Identification of environment types and adaptation zones with self-organizing maps; applications to sunflower multi-environment data in Europe. Theoretical and Applied Genetics, 2022, 135, 2059-2082.	1.8	8
100	Robust detection methodology of milk heat treatment in cheese based on volatile profile fingerprinting. International Dairy Journal, 2018, 85, 211-218.	1.5	5
101	Prediction of a suitable mobile phase composition in reversed-phase high-performance liquid chromatography using fragmental constants. Chemometrics and Intelligent Laboratory Systems, 1994, 25, 341-354.	1.8	4
102	Pinpointing Biomarkers in Proteomic LC/MS Data by Moving-Window Discriminant Analysis. Analytical Chemistry, 2011, 83, 5197-5206.	3.2	4
103	SMIXTURE: strategy for mixture model clustering of multivariate images. Journal of Chemometrics, 2005, 19, 607-614.	0.7	3
104	Detection of Tomato Flowers from Greenhouse Images Using Colorspace Transformations. Lecture Notes in Computer Science, 2019, , 146-155.	1.0	3
105	4: Expert-System-Development Tools. Data Handling in Science and Technology, 1993, 13, 121-151.	3.1	2
106	Calcium Imaging of GPCR Activation Using Arrays of Reverse Transfected HEK293 Cells in a Microfluidic System. Sensors, 2018, 18, 602.	2.1	2
107	Statistical models discriminating between complex samples measured with microfluidic receptor-cell arrays. PLoS ONE, 2019, 14, e0214878.	1.1	2
108	Metabolic Biomarker Identification with Few Samples. , 0, , .		2

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109	A computational model to predict clathration of molecules with cephradineâ€. Perkin Transactions II RSC, 2001, , 981-987.	1.1	1
110	On the maximization of likelihoods belonging to the exponential family using a Levenbergâ€“Marquardt approach. Journal of Statistical Computation and Simulation, 2017, 87, 895-907.	0.7	1
111	Ayurvedic Herbal Preparation Supplementation Does Not Improve Metabolic Health in Impaired Glucose Tolerance Subjects; Observations from a Randomised Placebo Controlled Trial. Nutrients, 2021, 13, 260.	1.7	1
112	Self-Organising Maps for Image Segmentation. Studies in Classification, Data Analysis, and Knowledge Organization, 2009, , 373-383.	0.1	1
113	7: Inductive Expert Systems. Data Handling in Science and Technology, 1993, 13, 261-279.	3.1	0
114	Chemometric Methods in Nuclear Magnetic Resonanceâ€“Based Body Fluid Analysis. , 0, , 244-256.		0
115	The Effect of Calcium Buffering and Calcium Sensor Type on the Sensitivity of an Array-Based Bitter Receptor Screening Assay. Chemical Senses, 2019, 44, 497-505.	1.1	0