

Ron Wehrens

List of Publications by Year in descending order

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115
papers

6,476
citations

76326

40
h-index

71685

76
g-index

120
all docs

120
docs citations

120
times ranked

10003
citing authors

#	ARTICLE	IF	CITATIONS
1	The pls Package: Principal Component and Partial Least Squares Regression in <i>R</i> . Journal of Statistical Software, 2007, 18, .	3.7	1,047
2	Self- and Super-organizing Maps in <i>R</i> : The kohonen Package. Journal of Statistical Software, 2007, 21, .	3.7	465
3	The bootstrap: a tutorial. Chemometrics and Intelligent Laboratory Systems, 2000, 54, 35-52.	3.5	399
4	Possibilities of visible–near-infrared spectroscopy for the assessment of soil contamination in river floodplains. Analytica Chimica Acta, 2001, 446, 97-105.	5.4	202
5	Chemometrics with R. , 2011, , .		187
6	Flexible Self-Organizing Maps in kohonen 3.0. Journal of Statistical Software, 2018, 87, .	3.7	183
7	Supervised Kohonen networks for classification problems. Chemometrics and Intelligent Laboratory Systems, 2006, 83, 99-113.	3.5	174
8	Improved batch correction in untargeted MS-based metabolomics. Metabolomics, 2016, 12, 88.	3.0	167
9	Exploring field vegetation reflectance as an indicator of soil contamination in river floodplains. Environmental Pollution, 2004, 127, 281-290.	7.5	156
10	The potential of field spectroscopy for the assessment of sediment properties in river floodplains. Analytica Chimica Acta, 2003, 484, 189-200.	5.4	129
11	A generalized expression for the similarity of spectra: application to powder diffraction pattern classification. Journal of Computational Chemistry, 2001, 22, 273-289.	3.3	112
12	Tomato Fruit Detection and Counting in Greenhouses Using Deep Learning. Frontiers in Plant Science, 2020, 11, 571299.	3.6	104
13	KNN-kernel density-based clustering for high-dimensional multivariate data. Computational Statistics and Data Analysis, 2006, 51, 513-525.	1.2	99
14	Identification of novel functional TBP-binding sites and general factor repertoires. EMBO Journal, 2007, 26, 944-954.	7.8	97
15	The WEIZMASS spectral library for high-confidence metabolite identification. Nature Communications, 2016, 7, 12423.	12.8	95
16	Flash Chemistry Extensively Optimized: High-Temperature Swern–Moffatt Oxidation in an Automated Microreactor Platform. Chemistry - an Asian Journal, 2010, 5, 799-805.	3.3	83
17	Identification of Novel Regulators Associated With Early-Phase Osteoblast Differentiation. Journal of Bone and Mineral Research, 2004, 19, 947-958.	2.8	82
18	Clustering multispectral images: a tutorial. Chemometrics and Intelligent Laboratory Systems, 2005, 77, 3-17.	3.5	82

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19	Multivariate statistical process control using mixture modelling. <i>Journal of Chemometrics</i> , 2005, 19, 23-31.	1.3	81
20	Evolutionary optimisation: a tutorial. <i>TrAC - Trends in Analytical Chemistry</i> , 1998, 17, 193-203.	11.4	80
21	Direct determination of molecular constants from rovibronic spectra with genetic algorithms. <i>Journal of Chemical Physics</i> , 2000, 113, 7955-7962.	3.0	77
22	Assessment of techniques for DOSY NMR data processing. <i>Analytica Chimica Acta</i> , 2003, 490, 231-251.	5.4	77
23	H, C, N and S stable isotopes and mineral profiles to objectively guarantee the authenticity of grated hard cheeses. <i>Analytica Chimica Acta</i> , 2012, 711, 54-59.	5.4	77
24	metaMS: An open-source pipeline for GC-MS-based untargeted metabolomics. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2014, 966, 109-116.	2.3	76
25	Warping methods for spectroscopic and chromatographic signal alignment: A tutorial. <i>Analytica Chimica Acta</i> , 2013, 781, 14-32.	5.4	75
26	LC-MS based global metabolite profiling of grapes: solvent extraction protocol optimisation. <i>Metabolomics</i> , 2012, 8, 175-185.	3.0	72
27	Interpretation of ANOVA models for microarray data using PCA. <i>Bioinformatics</i> , 2007, 23, 184-190.	4.1	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 <i>Picea abies</i> as climate proxies. <i>Rapid Communications in Mass Spectrometry</i> , 2013, 27, 265-275.	1.5	68
30	Improved parametric time warping for proteomics. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2010, 104, 65-74.	3.5	65
31	Incremental Model-Based Clustering for Large Datasets With Small Clusters. <i>Journal of Computational and Graphical Statistics</i> , 2005, 14, 529-546.	1.7	57
32	Model-Based Clustering for Image Segmentation and Large Datasets via Sampling. <i>Journal of Classification</i> , 2004, 21, 231-253.	2.2	55
33	Climatic and geographical dependence of the H, C and O stable isotope ratios of Italian wine. <i>Analytica Chimica Acta</i> , 2015, 853, 384-390.	5.4	55
34	The use of IRMS, ¹ H NMR and chemical analysis to characterise Italian and imported Tunisian olive oils. <i>Food Chemistry</i> , 2016, 196, 98-105.	8.2	55
35	Improved DOSY NMR data processing by data enhancement and combination of multivariate curve resolution with non-linear least square fitting. <i>Journal of Magnetic Resonance</i> , 2004, 169, 257-269.	2.1	54
36	A comparison of methods to relate grass reflectance to soil metal contamination. <i>International Journal of Remote Sensing</i> , 2003, 24, 4995-5010.	2.9	49

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37	A Procedure for Incorporating Spatial Variability in Ecological Risk Assessment of Dutch River Floodplains. <i>Environmental Management</i> , 2001, 28, 359-373.	2.7	48
38	Stability-based biomarker selection. <i>Analytica Chimica Acta</i> , 2011, 705, 15-23.	5.4	47
39	A targeted metabolomics approach to understand differences in flavonoid biosynthesis in red and yellow raspberries. <i>Plant Physiology and Biochemistry</i> , 2013, 72, 79-86.	5.8	47
40	Wavelength selection with Tabu Search. <i>Journal of Chemometrics</i> , 2003, 17, 427-437.	1.3	44
41	Spatial Variability and Uncertainty in Ecological Risk Assessment: A Case Study on the Potential Risk of Cadmium for the Little Owl in a Dutch River Flood Plain. <i>Environmental Science & Technology</i> , 2005, 39, 2177-2187.	10.0	42
42	Detecting the addition of sugar and water to wine. <i>Australian Journal of Grape and Wine Research</i> , 2013, 19, 324-330.	2.1	41
43	Initialization of Markov random field clustering of large remote sensing images. <i>IEEE Transactions on Geoscience and Remote Sensing</i> , 2005, 43, 1912-1919.	6.3	40
44	Traceability along the production chain of Italian tomato products on the basis of stable isotopes and mineral composition. <i>Rapid Communications in Mass Spectrometry</i> , 2011, 25, 899-909.	1.5	40
45	SpaRef: a clustering algorithm for multispectral images. <i>Analytica Chimica Acta</i> , 2003, 490, 303-312.	5.4	39
46	Method for the computational comparison of crystal structures. <i>Acta Crystallographica Section B: Structural Science</i> , 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 "Pinot noir"™ Vineyard. <i>Journal of Agricultural and Food Chemistry</i> , 2013, 61, 8976-8986.	5.2	36
48	Fast parametric time warping of peak lists. <i>Bioinformatics</i> , 2015, 31, 3063-3065.	4.1	33
49	A benchmark spike-in data set for biomarker identification in metabolomics. <i>Journal of Chemometrics</i> , 2012, 26, 16-24.	1.3	32
50	Sequential assignment of 2D-NMR spectra of proteins using genetic algorithms. <i>Journal of Chemical Information and Computer Sciences</i> , 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. <i>BMC Genomics</i> , 2014, 15, 1030.	2.8	31
52	Metabolite variation in the lettuce gene pool: towards healthier crop varieties and food. <i>Metabolomics</i> , 2018, 14, 146.	3.0	31
53	Linking GC-MS and PTR-TOF-MS fingerprints of food samples. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2012, 118, 301-307.	3.5	30
54	Statistical methods for improving verification of claims of origin for Italian wines based on stable isotope ratios. <i>Analytica Chimica Acta</i> , 2012, 757, 19-25.	5.4	29

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55	MetaDB a Data Processing Workflow in Untargeted MS-Based Metabolomics Experiments. <i>Frontiers in Bioengineering and Biotechnology</i> , 2014, 2, 72.	4.1	29
56	Using genetic algorithms for the construction of phylogenetic trees: application to G-protein coupled receptor sequences. <i>BioSystems</i> , 1999, 49, 31-43.	2.0	28
57	HIPS, a hybrid self-adapting expert system for nuclear magnetic resonance spectrum interpretation using genetic algorithms. <i>Analytica Chimica Acta</i> , 1993, 277, 313-324.	5.4	26
58	Constructing a mass measurement error surface to improve automatic annotations in liquid chromatography/mass spectrometry based metabolomics. <i>Rapid Communications in Mass Spectrometry</i> , 2013, 27, 2425-2431.	1.5	25
59	On the Use of ¹ H and ¹³ C 1D NMR Spectra as QSPR Descriptors. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 487-494.	5.4	23
60	Quality Criteria of Genetic Algorithms for Structure Optimization. <i>Journal of Chemical Information and Computer Sciences</i> , 1998, 38, 151-157.	2.8	22
61	The quality of optimisation by genetic algorithms. <i>Analytica Chimica Acta</i> , 1999, 388, 265-271.	5.4	22
62	Hybrid genetic algorithm-tabu search approach for optimising multilayer optical coatings. <i>Analytica Chimica Acta</i> , 2003, 490, 211-222.	5.4	22
63	Mixture modelling of medical magnetic resonance data. <i>Journal of Chemometrics</i> , 2002, 16, 274-282.	1.3	21
64	Stable isotope ratios of H, C, N and O in Italian citrus juices. <i>Journal of Mass Spectrometry</i> , 2014, 49, 785-791.	1.6	21
65	Self-organizing maps: A versatile tool for the automatic analysis of untargeted imaging datasets. <i>Proteomics</i> , 2014, 14, 853-861.	2.2	21
66	High-throughput carotenoid profiling using multivariate curve resolution. <i>Analytical and Bioanalytical Chemistry</i> , 2013, 405, 5075-5086.	3.7	20
67	Multiple comparisons in mass-spectrometry-based -omics technologies. <i>TrAC - Trends in Analytical Chemistry</i> , 2013, 50, 11-21.	11.4	20
68	Molecular data-mining: a challenge for chemometrics. <i>Chemometrics and Intelligent Laboratory Systems</i> , 1999, 49, 121-133.	3.5	18
69	Real-life applications of the MULVADO software package for processing DOSY NMR data. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, 110-117.	1.9	18
70	The Influence of Different Structure Representations on the Clustering of an RNA Nucleotides Data Set. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 1388-1394.	2.8	16
71	Powder pattern indexing using the weighted crosscorrelation and genetic algorithms. <i>Journal of Computational Chemistry</i> , 2003, 24, 1043-1051.	3.3	15
72	Integrating gene expression and GO classification for PCA by preclustering. <i>BMC Bioinformatics</i> , 2010, 11, 158.	2.6	15

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73	Automatic Phenotyping of Tomatoes in Production Greenhouses Using Robotics and Computer Vision: From Theory to Practice. <i>Agronomy</i> , 2021, 11, 1599.	3.0	15
74	Robust ANOVA for microarray data. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2009, 98, 38-44.	3.5	14
75	F1 hybrid of cultivated apple (<i>Malus domestica</i>) and European pear (<i>Pyrus communis</i>) with fertile F2 offspring. <i>Molecular Breeding</i> , 2014, 34, 817-828.	2.1	14
76	Oxygen and Hydrogen Stable Isotope Ratios of Bulk Needles Reveal the Geographic Origin of Norway Spruce in the European Alps. <i>PLoS ONE</i> , 2015, 10, e0118941.	2.5	14
77	Meta-Statistics for Variable Selection: The <i>R</i> Package <i>BioMark</i> . <i>Journal of Statistical Software</i> , 2012, 51, .	3.7	14
78	Circular effects in representations of an RNA nucleotides data set in relation with principal components analysis. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2001, 56, 61-71.	3.5	13
79	Robust DOSY NMR data analysis. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2007, 85, 9-19.	3.5	13
80	Sampling of aquatic sediments. Designs of a decision-support system and a case study. <i>Analytica Chimica Acta</i> , 1993, 271, 11-24.	5.4	12
81	Calibration of an array of voltammetric microelectrodes. <i>Analytica Chimica Acta</i> , 1996, 334, 93-101.	5.4	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. <i>Journal of Magnetic Resonance</i> , 2005, 172, 346-358.	2.1	12
84	D-optimal design of an untargeted HS-SPME-GC-TOF metabolite profiling method. <i>Analyst</i> , The, 2012, 137, 3725.	3.5	12
85	A comprehensive full factorial <i>LC-MS/MS</i> proteomics benchmark data set. <i>Proteomics</i> , 2012, 12, 2276-2281.	2.2	12
86	Metabolite profiling in LC-DAD using multivariate curve resolution: the alsace package for R. <i>Metabolomics</i> , 2015, 11, 143-154.	3.0	12
87	Possibilities of soil spectroscopy for the classification of contaminated areas in river floodplains. <i>International Journal of Applied Earth Observation and Geoinformation</i> , 2001, 3, 337-344.	2.8	11
88	Chemometrics with R. Use R!, 2020, , .	0.2	11
89	Representing structural databases in a self-organizing map. <i>Acta Crystallographica Section B: Structural Science</i> , 2005, 61, 548-557.	1.8	10
90	Thresholding for biomarker selection in multivariate data using Higher Criticism. <i>Molecular BioSystems</i> , 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. <i>Scientific Data</i> , 2021, 8, 52.	5.3	10
92	A controlled human intervention trial to study protein quality by amino acid uptake kinetics with the novel <i>Lemna</i> protein concentrate as case study. <i>International Journal of Food Sciences and Nutrition</i> , 2022, 73, 251-262.	2.8	10
93	Supervised Self-Organizing Maps in Crystal Property and Structure Prediction. <i>Crystal Growth and Design</i> , 2007, 7, 1738-1745.	3.0	9
94	Effects of climate change on the distribution of crop wild relatives in the Netherlands in relation to conservation status and ecotope variation. <i>Global Ecology and Conservation</i> , 2020, 23, e01054.	2.1	9
95	Validation and refinement of expert systems: interpretation of NMR spectra as an application in analytical chemistry. <i>Chemometrics and Intelligent Laboratory Systems</i> , 1991, 12, 57-67.	3.5	8
96	Molecular challenges in modern chemometrics. <i>Analytica Chimica Acta</i> , 1999, 400, 413-424.	5.4	8
97	Molecular Chemometrics. <i>Critical Reviews in Analytical Chemistry</i> , 2006, 36, 189-198.	3.5	8
98	Glucosinolate variability between turnip organs during development. <i>PLoS ONE</i> , 2019, 14, e0217862.	2.5	8
99	Identification of environment types and adaptation zones with self-organizing maps; applications to sunflower multi-environment data in Europe. <i>Theoretical and Applied Genetics</i> , 2022, 135, 2059-2082.	3.6	8
100	Robust detection methodology of milk heat treatment in cheese based on volatile profile fingerprinting. <i>International Dairy Journal</i> , 2018, 85, 211-218.	3.0	5
101	Prediction of a suitable mobile phase composition in reversed-phase high-performance liquid chromatography using fragmental constants. <i>Chemometrics and Intelligent Laboratory Systems</i> , 1994, 25, 341-354.	3.5	4
102	Pinpointing Biomarkers in Proteomic LC/MS Data by Moving-Window Discriminant Analysis. <i>Analytical Chemistry</i> , 2011, 83, 5197-5206.	6.5	4
103	SMIXTURE: strategy for mixture model clustering of multivariate images. <i>Journal of Chemometrics</i> , 2005, 19, 607-614.	1.3	3
104	Detection of Tomato Flowers from Greenhouse Images Using Colorspace Transformations. <i>Lecture Notes in Computer Science</i> , 2019, , 146-155.	1.3	3
105	4: Expert-System-Development Tools. <i>Data Handling in Science and Technology</i> , 1993, 13, 121-151.	3.1	2
106	Calcium Imaging of GPCR Activation Using Arrays of Reverse Transfected HEK293 Cells in a Microfluidic System. <i>Sensors</i> , 2018, 18, 602.	3.8	2
107	Statistical models discriminating between complex samples measured with microfluidic receptor-cell arrays. <i>PLoS ONE</i> , 2019, 14, e0214878.	2.5	2
108	Metabolic Biomarker Identification with Few Samples. , 0, , .		2

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109	A computational model to predict clathration of molecules with cephradine. Perkin Transactions II RSC, 2001, , 981-987.	1.1	1
110	On the maximization of likelihoods belonging to the exponential family using a Levenberg-Marquardt approach. Journal of Statistical Computation and Simulation, 2017, 87, 895-907.	1.2	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.	4.1	1
112	Self-Organising Maps for Image Segmentation. Studies in Classification, Data Analysis, and Knowledge Organization, 2009, , 373-383.	0.2	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 Resonance-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.	2.0	0