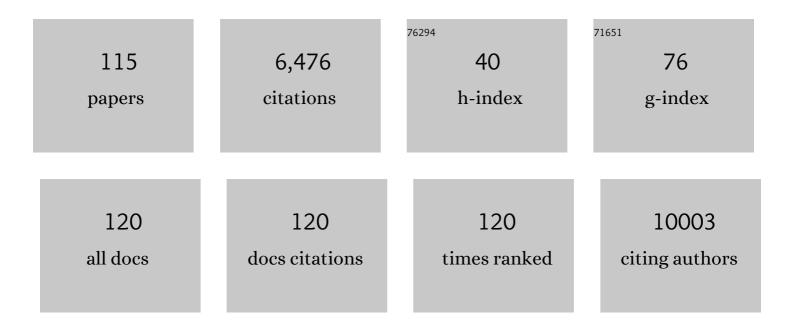
List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	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
2	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
3	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
4	LC-MS based plant metabolic profiles of thirteen grassland species grown in diverse neighbourhoods. Scientific Data, 2021, 8, 52.	2.4	10
5	Automatic Phenotyping of Tomatoes in Production Greenhouses Using Robotics and Computer Vision: From Theory to Practice. Agronomy, 2021, 11, 1599.	1.3	15
6	Chemometrics with R. Use R!, 2020, , .	0.3	11
7	Tomato Fruit Detection and Counting in Greenhouses Using Deep Learning. Frontiers in Plant Science, 2020, 11, 571299.	1.7	104
8	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
9	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
10	Glucosinolate variability between turnip organs during development. PLoS ONE, 2019, 14, e0217862.	1.1	8
11	Statistical models discriminating between complex samples measured with microfluidic receptor-cell arrays. PLoS ONE, 2019, 14, e0214878.	1.1	2
12	Detection of Tomato Flowers from Greenhouse Images Using Colorspace Transformations. Lecture Notes in Computer Science, 2019, , 146-155.	1.0	3
13	Metabolite variation in the lettuce gene pool: towards healthier crop varieties and food. Metabolomics, 2018, 14, 146.	1.4	31
14	Robust detection methodology of milk heat treatment in cheese based on volatile profile fingerprinting. International Dairy Journal, 2018, 85, 211-218.	1.5	5
15	Calcium Imaging of GPCR Activation Using Arrays of Reverse Transfected HEK293 Cells in a Microfluidic System. Sensors, 2018, 18, 602.	2.1	2
16	Flexible Self-Organizing Maps in kohonen 3.0. Journal of Statistical Software, 2018, 87, .	1.8	183
17	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.	0.7	1
18	The WEIZMASS spectral library for high-confidence metabolite identification. Nature Communications, 2016, 7, 12423.	5.8	95

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19	Improved batch correction in untargeted MS-based metabolomics. Metabolomics, 2016, 12, 88.	1.4	167
20	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
21	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
22	Metabolite profiling in LC–DAD using multivariate curve resolution: the alsace package for R. Metabolomics, 2015, 11, 143-154.	1.4	12
23	Fast parametric time warping of peak lists. Bioinformatics, 2015, 31, 3063-3065.	1.8	33
24	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
25	MetaDB a Data Processing Workflow in Untargeted MS-Based Metabolomics Experiments. Frontiers in Bioengineering and Biotechnology, 2014, 2, 72.	2.0	29
26	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
27	Stable isotope ratios of H, C, N and O in Italian citrus juices. Journal of Mass Spectrometry, 2014, 49, 785-791.	0.7	21
28	Selfâ€organizing maps: A versatile tool for the automatic analysis of untargeted imaging datasets. Proteomics, 2014, 14, 853-861.	1.3	21
29	metaMS: An open-source pipeline for GC–MS-based untargeted metabolomics. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2014, 966, 109-116.	1.2	76
30	F1 hybrid of cultivated apple (MalusÂ×Âdomestica) and European pear (Pyrus communis) with fertile F2 offspring. Molecular Breeding, 2014, 34, 817-828.	1.0	14
31	High-throughput carotenoid profiling using multivariate curve resolution. Analytical and Bioanalytical Chemistry, 2013, 405, 5075-5086.	1.9	20
32	Use of Metabolic Profiling To Study Grape Skin Polyphenol Behavior as a Result of Canopy Microclimate Manipulation in a †Pinot noir' Vineyard. Journal of Agricultural and Food Chemistry, 2013, 61, 8976-8986.	2.4	36
33	Carbon, hydrogen and oxygen stable isotope ratios of whole wood, cellulose and lignin methoxyl groups of <i>Picea abies</i> as climate proxies. Rapid Communications in Mass Spectrometry, 2013, 27, 265-275.	0.7	68
34	Detecting the addition of sugar and water to wine. Australian Journal of Grape and Wine Research, 2013, 19, 324-330.	1.0	41
35	Multiple comparisons in mass-spectrometry-based -omics technologies. TrAC - Trends in Analytical Chemistry, 2013, 50, 11-21.	5.8	20
36	Warping methods for spectroscopic and chromatographic signal alignment: A tutorial. Analytica Chimica Acta, 2013, 781, 14-32.	2.6	75

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37	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
38	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
39	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
40	Thresholding for biomarker selection in multivariate data using Higher Criticism. Molecular BioSystems, 2012, 8, 2339.	2.9	10
41	Linking GC-MS and PTR-TOF-MS fingerprints of food samples. Chemometrics and Intelligent Laboratory Systems, 2012, 118, 301-307.	1.8	30
42	D-optimal design of an untargeted HS-SPME-GC-TOF metabolite profiling method. Analyst, The, 2012, 137, 3725.	1.7	12
43	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
44	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
45	LC-MS based global metabolite profiling of grapes: solvent extraction protocol optimisation. Metabolomics, 2012, 8, 175-185.	1.4	72
46	A benchmark spikeâ€in data set for biomarker identification in metabolomics. Journal of Chemometrics, 2012, 26, 16-24.	0.7	32
47	Meta-Statistics for Variable Selection: The <i>R</i> Package BioMark . Journal of Statistical Software, 2012, 51, .	1.8	14
48	Pinpointing Biomarkers in Proteomic LC/MS Data by Moving-Window Discriminant Analysis. Analytical Chemistry, 2011, 83, 5197-5206.	3.2	4
49	Stability-based biomarker selection. Analytica Chimica Acta, 2011, 705, 15-23.	2.6	47
50	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
51	Chemometrics with R., 2011, , .		187
52	Flash Chemistry Extensively Optimized: Highâ€īemperature Swern–Moffatt Oxidation in an Automated Microreactor Platform. Chemistry - an Asian Journal, 2010, 5, 799-805.	1.7	83
53	Integrating gene expression and GO classification for PCA by preclustering. BMC Bioinformatics, 2010, 11, 158.	1.2	15
54	Improved parametric time warping for proteomics. Chemometrics and Intelligent Laboratory Systems, 2010, 104, 65-74.	1.8	65

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55	Robust ANOVA for microarray data. Chemometrics and Intelligent Laboratory Systems, 2009, 98, 38-44.	1.8	14
56	Self-Organising Maps for Image Segmentation. Studies in Classification, Data Analysis, and Knowledge Organization, 2009, , 373-383.	0.1	1
57	Interpretation of ANOVA models for microarray data using PCA. Bioinformatics, 2007, 23, 184-190.	1.8	70
58	Supervised Self-Organizing Maps in Crystal Property and Structure Prediction. Crystal Growth and Design, 2007, 7, 1738-1745.	1.4	9
59	Robust DOSY NMR data analysis. Chemometrics and Intelligent Laboratory Systems, 2007, 85, 9-19.	1.8	13
60	Identification of novel functional TBP-binding sites and general factor repertoires. EMBO Journal, 2007, 26, 944-954.	3.5	97
61	The pls Package: Principal Component and Partial Least Squares Regression in <i>R</i> . Journal of Statistical Software, 2007, 18, .	1.8	1,047
62	Self- and Super-organizing Maps in <i>R</i> : The kohonen Package. Journal of Statistical Software, 2007, 21, .	1.8	465
63	Molecular Chemometrics. Critical Reviews in Analytical Chemistry, 2006, 36, 189-198.	1.8	8
64	On the Use of1H and13C 1D NMR Spectra as QSPR Descriptors. Journal of Chemical Information and Modeling, 2006, 46, 487-494.	2.5	23
65	KNN-kernel density-based clustering for high-dimensional multivariate data. Computational Statistics and Data Analysis, 2006, 51, 513-525.	0.7	99
66	Supervised Kohonen networks for classification problems. Chemometrics and Intelligent Laboratory Systems, 2006, 83, 99-113.	1.8	174
67	Real-life applications of the MULVADO software package for processing DOSY NMR data. Magnetic Resonance in Chemistry, 2006, 44, 110-117.	1.1	18
68	Clustering multispectral images: a tutorial. Chemometrics and Intelligent Laboratory Systems, 2005, 77, 3-17.	1.8	82
69	Incremental Model-Based Clustering for Large Datasets With Small Clusters. Journal of Computational and Graphical Statistics, 2005, 14, 529-546.	0.9	57
70	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
71	Multivariate statistical process control using mixture modelling. Journal of Chemometrics, 2005, 19, 23-31.	0.7	81
72	SMIXTURE: strategy for mixture model clustering of multivariate images. Journal of Chemometrics, 2005, 19, 607-614.	0.7	3

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73	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
74	Method for the computational comparison of crystal structures. Acta Crystallographica Section B: Structural Science, 2005, 61, 29-36.	1.8	36
75	Representing structural databases in a self-organizing map. Acta Crystallographica Section B: Structural Science, 2005, 61, 548-557.	1.8	10
76	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
77	Identification of Novel Regulators Associated With Early-Phase Osteoblast Differentiation. Journal of Bone and Mineral Research, 2004, 19, 947-958.	3.1	82
78	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
79	Model-Based Clustering for Image Segmentation and Large Datasets via Sampling. Journal of Classification, 2004, 21, 231-253.	1.2	55
80	Exploring field vegetation reflectance as an indicator of soil contamination in river floodplains. Environmental Pollution, 2004, 127, 281-290.	3.7	156
81	Powder pattern indexing using the weighted crosscorrelation and genetic algorithms. Journal of Computational Chemistry, 2003, 24, 1043-1051.	1.5	15
82	Wavelength selection with Tabu Search. Journal of Chemometrics, 2003, 17, 427-437.	0.7	44
83	The potential of field spectroscopy for the assessment of sediment properties in river floodplains. Analytica Chimica Acta, 2003, 484, 189-200.	2.6	129
84	SpaRef: a clustering algorithm for multispectral images. Analytica Chimica Acta, 2003, 490, 303-312.	2.6	39
85	Assessment of techniques for DOSY NMR data processing. Analytica Chimica Acta, 2003, 490, 231-251.	2.6	77
86	Hybrid genetic algorithm–tabu search approach for optimising multilayer optical coatings. Analytica Chimica Acta, 2003, 490, 211-222.	2.6	22
87	A comparison of methods to relate grass reflectance to soil metal contamination. International Journal of Remote Sensing, 2003, 24, 4995-5010.	1.3	49
88	Mixture modelling of medical magnetic resonance data. Journal of Chemometrics, 2002, 16, 274-282.	0.7	21
89	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
90	A computational model to predict clathration of molecules with cephradineâ€. Perkin Transactions II RSC, 2001, , 981-987.	1.1	1

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91	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
92	A Procedure for Incorporating Spatial Variability in Ecological Risk Assessment of Dutch River Floodplains. Environmental Management, 2001, 28, 359-373.	1.2	48
93	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
94	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
95	Possibilities of visible–near-infrared spectroscopy for the assessment of soil contamination in river floodplains. Analytica Chimica Acta, 2001, 446, 97-105.	2.6	202
96	The bootstrap: a tutorial. Chemometrics and Intelligent Laboratory Systems, 2000, 54, 35-52.	1.8	399
97	Direct determination of molecular constants from rovibronic spectra with genetic algorithms. Journal of Chemical Physics, 2000, 113, 7955-7962.	1.2	77
98	Using genetic algorithms for the construction of phylogenetic trees: application to G-protein coupled receptor sequences. BioSystems, 1999, 49, 31-43.	0.9	28
99	Molecular data-mining: a challenge for chemometrics. Chemometrics and Intelligent Laboratory Systems, 1999, 49, 121-133.	1.8	18
100	The quality of optimisation by genetic algorithms. Analytica Chimica Acta, 1999, 388, 265-271.	2.6	22
101	Molecular challenges in modern chemometrics. Analytica Chimica Acta, 1999, 400, 413-424.	2.6	8
102	Quality criteria of genetic algorithms for construction of phylogenetic trees. , 1999, 20, 867-876.		12
103	Evolutionary optimisation: a tutorial. TrAC - Trends in Analytical Chemistry, 1998, 17, 193-203.	5.8	80
104	Quality Criteria of Genetic Algorithms for Structure Optimization. Journal of Chemical Information and Computer Sciences, 1998, 38, 151-157.	2.8	22
105	Bootstrapping principal component regression models. , 1997, 11, 157-171.		68
106	Calibration of an array of voltammetric microelectrodes. Analytica Chimica Acta, 1996, 334, 93-101.	2.6	12
107	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
108	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

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109	Sampling of aquatic sediments. Designs of a decision-support system and a case study. Analytica Chimica Acta, 1993, 271, 11-24.	2.6	12
110	4: Expert-System-Development Tools. Data Handling in Science and Technology, 1993, 13, 121-151.	3.1	2
111	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
112	7: Inductive Expert Systems. Data Handling in Science and Technology, 1993, 13, 261-279.	3.1	0
113	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
114	Chemometric Methods in Nuclear Magnetic Resonance–Based Body Fluid Analysis. , 0, , 244-256.		0
115	Metabolic Biomarker Identification with Few Samples. , 0, , .		2