Beata Walczak

List of Publications by Year
in descending order

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100 papers	5,371 citations	81743 39 h-index	82410 72 g-index
103 all docs	103 docs citations	103 times ranked	4872 citing authors

#	Article	IF	Citations
1	Particle swarm optimization (PSO). A tutorial. Chemometrics and Intelligent Laboratory Systems, 2015, 149, 153-165.	1.8	885
2	Representative subset selection. Analytica Chimica Acta, 2002, 468, 91-103.	2.6	254
3	Comparison of regularized discriminant analysis linear discriminant analysis and quadratic discriminant analysis applied to NIR data. Analytica Chimica Acta, 1996, 329, 257-265.	2.6	198
4	A comparison of two algorithms for warping of analytical signals. Analytica Chimica Acta, 2002, 456, 77-92.	2.6	195
5	The Radial Basis Functions â€" Partial Least Squares approach as a flexible non-linear regression technique. Analytica Chimica Acta, 1996, 331, 177-185.	2.6	192
6	TOMCAT: A MATLAB toolbox for multivariate calibration techniques. Chemometrics and Intelligent Laboratory Systems, 2007, 85, 269-277.	1.8	170
7	Raman spectroscopy as a process analytical technology (PAT) tool for the in-line monitoring and understanding of a powder blending process. Journal of Pharmaceutical and Biomedical Analysis, 2008, 48, 772-779.	1.4	132
8	Tracing the geographical origin of honeys based on volatile compounds profiles assessment using pattern recognition techniques. Food Chemistry, 2010, 118, 171-176.	4.2	132
9	Application of Wavelet Packet Transform in Pattern Recognition of Near-IR Data. Analytical Chemistry, 1996, 68, 1742-1747.	3.2	117
10	Comparison of multivariate methods based on latent vectors and methods based on wavelength selection for the analysis of near-infrared spectroscopic data. Analytica Chimica Acta, 1995, 304, 285-295.	2.6	114
11	Application of Wavelet Transform To Extract the Relevant Component from Spectral Data for Multivariate Calibration. Analytical Chemistry, 1997, 69, 4317-4323.	3.2	109
12	Dealing with missing values and outliers in principal component analysis. Talanta, 2007, 72, 172-178.	2.9	105
13	Chemometrics in analytical chemistryâ€"part II: modeling, validation, and applications. Analytical and Bioanalytical Chemistry, 2018, 410, 6691-6704.	1.9	102
14	Spectral transformation and wavelength selection in near-infrared spectra classification. Analytica Chimica Acta, 1995, 315, 243-255.	2.6	101
15	Use and abuse of chemometrics in chromatography. TrAC - Trends in Analytical Chemistry, 2006, 25, 1081-1096.	5.8	101
16	Chemometrics in analytical chemistryâ€"part I: history, experimental design and data analysis tools. Analytical and Bioanalytical Chemistry, 2017, 409, 5891-5899.	1.9	95
17	Fuzzy warping of chromatograms. Chemometrics and Intelligent Laboratory Systems, 2005, 77, 173-180.	1.8	91
18	Looking for Natural Patterns in Analytical Data. 2. Tracing Local Density with OPTICS. Journal of Chemical Information and Computer Sciences, 2002, 42, 500-507.	2.8	88

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19	The comparative molecular surface analysis (COMSA): a novel tool for molecular design. Computers & Chemistry, 2000, 24, 615-625.	1.2	87
20	Wavelets â€" something for analytical chemistry?. TrAC - Trends in Analytical Chemistry, 1997, 16, 451-463.	5.8	86
21	What can go wrong at the data normalization step for identification of biomarkers?. Journal of Chromatography A, 2014, 1362, 194-205.	1.8	86
22	Comparison of Multivariate Calibration Techniques Applied to Experimental NIR Data Sets. Applied Spectroscopy, 2000, 54, 608-623.	1.2	81
23	The Use of Wavelets for Signal Denoising in Capillary Electrophoresis. Analytical Chemistry, 2001, 73, 4903-4917.	3.2	75
24	Application of Radial Basis Functions â€" Partial Least Squares to non-linear pattern recognition problems: diagnosis of process faults. Analytica Chimica Acta, 1996, 331, 187-193.	2.6	65
25	Peak Alignment of Urine NMR Spectra Using Fuzzy Warping. Journal of Chemical Information and Modeling, 2006, 46, 863-875.	2.5	62
26	Start-to-end processing of two-dimensional gel electrophoretic images. Journal of Chromatography A, 2007, 1158, 306-317.	1.8	60
27	VSN: Variable sorting for normalization. Journal of Chemometrics, 2020, 34, e3164.	0.7	59
28	Three-way principal component analysis applied to food analysis: an example. Analytica Chimica Acta, 2002, 462, 133-148.	2.6	57
29	Determination and speciation of trace and ultratrace selenium ions by energy-dispersive X-ray fluorescence spectrometry using graphene as solid adsorbent in dispersive micro-solid phase extraction. Talanta, 2015, 134, 360-365.	2.9	57
30	A Comparison of Positive Matrix Factorization and the Weighted Multivariate Curve Resolution Method. Application to Environmental Data. Environmental Science & Technology, 2011, 45, 10102-10110.	4.6	56
31	Robust partial least squares model for prediction of green tea antioxidant capacity from chromatograms. Journal of Chromatography A, 2007, 1176, 12-18.	1.8	53
32	Preprocessing of two-dimensional gel electrophoresis images. Proteomics, 2004, 4, 2377-2389.	1.3	52
33	About kernel latent variable approaches and SVM. Journal of Chemometrics, 2005, 19, 341-354.	0.7	51
34	Target selection for alignment of chromatographic signals obtained using monochannel detectors. Journal of Chromatography A, 2007, 1176, 1-11.	1.8	51
35	Near-infrared reflectance spectroscopy and multivariate calibration techniques applied to modelling the crude protein, fibre and fat content in rapeseed meal. Analyst, The, 2008, 133, 1523.	1.7	50
36	Analysis of variance of designed chromatographic data sets: The analysis of variance-target projection approach. Journal of Chromatography A, 2015, 1405, 94-102.	1.8	46

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37	Multiple factor analysis in environmental chemistry. Analytica Chimica Acta, 2005, 545, 1-12.	2.6	43
38	Instrumentation of a roll compactor and the evaluation of the parameter settings by neural networks. International Journal of Pharmaceutics, 1997, 148, 103-115.	2.6	41
39	Automated alignment of one-dimensional chromatographic fingerprints. Journal of Chromatography A, 2010, 1217, 6127-6133.	1.8	40
40	Non-linear modelling of chemical data by combinations of linear and neural net methods. Analytica Chimica Acta, 1993, 283, 508-517.	2.6	38
41	Pixelâ€based analysis of multiple images for the identification of changes: A novel approach applied to unravel proteome patters of 2â€D electrophoresis gel images. Proteomics, 2007, 7, 3450-3461.	1.3	38
42	Classification and Regression TreesStudies of HIV Reverse Transcriptase Inhibitors. Journal of Chemical Information and Computer Sciences, 2004, 44, 716-726.	2.8	37
43	Transfer of Calibrations of Near-Infrared Spectra Using Neural Networks. Applied Spectroscopy, 1998, 52, 732-745.	1.2	36
44	Factor analysis and experiment design in high-performance liquid chromatography. Journal of Chromatography A, 1987, 395, 183-202.	1.8	34
45	Concept of (dis)similarity in data analysis. TrAC - Trends in Analytical Chemistry, 2012, 38, 116-128.	5.8	33
46	Neural networks with robust backpropagation learning algorithm. Analytica Chimica Acta, 1996, 322, 21-29.	2.6	32
47	Feature Based Fuzzy Matching of 2D Gel Electrophoresis Images. Journal of Chemical Information and Computer Sciences, 2002, 42, 1431-1442.	2.8	32
48	On the Optimal Partitioning of Data with K-Means, Growing K-Means, Neural Gas, and Growing Neural Gas. Journal of Chemical Information and Computer Sciences, 2002, 42, 1378-1389.	2.8	32
49	Proteomic analysis of striatal neuronal cell cultures after morphine administration. Journal of Separation Science, 2009, 32, 1200-1210.	1.3	31
50	Calibration of somatic cell count in milk based on near-infrared spectroscopy. Analytica Chimica Acta, 2001, 450, 131-141.	2.6	29
51	The Proteomic Analysis of Primary Cortical Astrocyte Cell Culture after Morphine Administration. Journal of Proteome Research, 2009, 8, 4633-4640.	1.8	28
52	Maize proteomic responses to separate or overlapping soil drought and two-spotted spider mite stresses. Planta, 2016, 244, 939-960.	1.6	28
53	Factor analysis and experiment design in high-performance liquid chromatography. Journal of Chromatography A, 1986, 353, 109-121.	1.8	27
54	Factor analysis and experiment design in high-performance liquid chromatography. Journal of Chromatography A, 1986, 371, 253-267.	1.8	27

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55	A journey into low-dimensional spaces with autoassociative neural networks. Talanta, 2003, 59, 1095-1105.	2.9	27
56	Factor analysis and experiment design in high-performance liquid chromatography. Journal of Chromatography A, 1986, 353, 123-137.	1.8	26
57	Simultaneous optimisation of extraction of xanthone and benzophenone Î±-glucosidase inhibitors from Cyclopia genistoides and identification of superior genotypes for propagation. Journal of Functional Foods, 2017, 33, 21-31.	1.6	23
58	Feature reduction by Fourier transform in pattern recognition of NIR data. Analytica Chimica Acta, 1996, 331, 75-83.	2.6	22
59	Principal component analysis of dissolution data with missing elements. International Journal of Pharmaceutics, 2002, 234, 169-178.	2.6	21
60	Modeling of the total antioxidant capacity of rooibos (Aspalathus linearis) tea infusions from chromatographic fingerprints and identification of potential antioxidant markers. Journal of Chromatography A, 2014, 1366, 101-109.	1.8	21
61	How to construct a multiple regression model for data with missing elements and outlying objects. Analytica Chimica Acta, 2007, 581, 324-332.	2.6	20
62	Matching 2D Gel Electrophoresis Images. Journal of Chemical Information and Computer Sciences, 2003, 43, 978-986.	2.8	18
63	Phenolic composition of rooibos changes during simulated fermentation: Effect of endogenous enzymes and fermentation temperature on reaction kinetics. Food Research International, 2019, 121, 185-196.	2.9	18
64	A neuro-fuzzy system for X-ray spectra interpretation. Mikrochimica Acta, 1994, 113, 153-169.	2.5	17
65	Discrimination of biofilm samples using pattern recognition techniques. Analytical and Bioanalytical Chemistry, 2008, 390, 1273-1282.	1.9	17
66	Relating gas chromatographic profiles to sensory measurements describing the end products of the Maillard reaction. Talanta, 2011, 83, 1239-1246.	2.9	17
67	Classification of data with missing elements and outliersâˆ†. Talanta, 2008, 76, 602-609.	2.9	16
68	Robust biomarker identification in a two-class problem based on pairwise log-ratios. Chemometrics and Intelligent Laboratory Systems, 2017, 171, 277-285.	1.8	16
69	Again about partial least squares and feature selection. Chemometrics and Intelligent Laboratory Systems, 2012, 115, 9-17.	1.8	15
70	Classification of genomic data: Some aspects of feature selection. Talanta, 2008, 76, 564-574.	2.9	13
71	Multivariate analysis of variance of designed chromatographic data. A case study involving fermentation of rooibos tea. Journal of Chromatography A, 2017, 1489, 115-125.	1.8	13
72	Different strategies for class model optimization. A comparative study. Talanta, 2020, 215, 120912.	2.9	12

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73	Genotypic variation in phenolic composition of Cyclopia pubescens (honeybush tea) seedling plants. Journal of Food Composition and Analysis, 2019, 78, 129-137.	1.9	11
74	Authentication of honeybush and rooibos herbal teas based on their elemental composition. Food Control, 2021, 123, 107757.	2.8	9
75	High-temperature oxidation reduces the bitterness of honeybush infusions depending on changes in phenolic composition. LWT - Food Science and Technology, 2021, 139, 110608.	2.5	9
76	Non-parametric multivariate analysis of variance in the proteomic response of potato to drought stress. Analytica Chimica Acta, 2012, 719, 1-7.	2.6	8
77	Ultratrace determination of metal ions using graphene oxide/carbon nanotubes loaded cellulose membranes and total-reflection X-ray fluorescence spectrometry: A green chemistry approach. Spectrochimica Acta, Part B: Atomic Spectroscopy, 2021, 177, 106069.	1.5	8
78	Cellulose sorbents in investigations on self-association of higher fatty alcohols. Microchemical Journal, 1981, 26, 299-306.	2.3	7
79	Robust Methods in Analysis of Multivariate Food Chemistry Data. Data Handling in Science and Technology, 2013, , 315-340.	3.1	7
80	Model development for predicting in vitro bio-capacity of green rooibos extract based on composition for application as screening tool in quality control. Food and Function, 2020, 11, 3084-3094.	2.1	7
81	Class-modelling of overlapping classes. A two-step authentication approach. Analytica Chimica Acta, 2022, 1191, 339284.	2.6	7
82	Combining class-modelling and discriminant methods for improvement of products authentication. Chemometrics and Intelligent Laboratory Systems, 2022, 228, 104620.	1.8	7
83	Finding relevant clustering directions in highâ€dimensional data using Particle Swarm Optimization. Journal of Chemometrics, 2011, 25, 366-374.	0.7	6
84	SEPARATION OF CHALCONES ISOMERS IN HPLC SYSTEMS. Analytical Sciences, 1991, 7, 103-107.	0.8	5
85	The scope of applicability of the selected class-modelling methods. Chemometrics and Intelligent Laboratory Systems, 2021, 218, 104427.	1.8	5
86	Working with log-ratios. Analytica Chimica Acta, 2019, 1059, 16-27.	2.6	4
87	Chromatographic and spectroscopic investigation of the associative changes with the selected higher fatty alcohols. Microchemical Journal, 1980, 25, 330-337.	2.3	3
88	Wavelet Bases for IR Library Compression, Searching and Reconstruction. Data Handling in Science and Technology, 2000, 22, 291-310.	3.1	3
89	ANOVA-Target Projection (ANOVA-TP). , 2020, , 495-520.		3
90	Non-destructive elemental analysis of herbal teas from South Africa. Journal of Food Composition and Analysis, 2021, 102, 104041.	1.9	3

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91	European analytical column. TrAC - Trends in Analytical Chemistry, 2014, 56, ix-xii.	5.8	2
92	Untargeted analysis of chromatographic data for green and fermented rooibos: Problem with size effect removal. Journal of Chromatography A, 2017, 1525, 109-115.	1.8	2
93	Robust Methods in Qsar. Challenges and Advances in Computational Chemistry and Physics, 2010, , 177-208.	0.6	1
94	Investigation of the association of the 1-dodecene-lauryl alcohol bicomponent system. Microchemical Journal, 1981, 26, 590-596.	2.3	0
95	Estimation of the number of true null hypotheses when conducting a multiple testing. Chemometrics and Intelligent Laboratory Systems, 2010, 104, 281-288.	1.8	0
96	A new concept for variance analysis of hyphenated chromatographic data avoiding signal warping. Journal of Chromatography A, 2013, 1291, 64-72.	1.8	0
97	European Analytical Column Number 42. Journal of Analytical Chemistry, 2014, 69, 812-816.	0.4	0
98	European analytical column number 42. Accreditation and Quality Assurance, 2014, 19, 225-229.	0.4	0
99	Particle Swarm Optimization. , 2020, , 649-666.		0
100	Chemometria w metabolomice i proteomice. , 2010, , .		0