

# Beata Walczak

## List of Publications by Year in descending order

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Version: 2024-02-01

100  
papers

5,371  
citations

81900

39  
h-index

82547

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. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2015, 149, 153-165.   | 3.5  | 885       |
| 2  | Representative subset selection. <i>Analytica Chimica Acta</i> , 2002, 468, 91-103.   | 5.4  | 254       |
| 3  | Comparison of regularized discriminant analysis linear discriminant analysis and quadratic discriminant analysis applied to NIR data. <i>Analytica Chimica Acta</i> , 1996, 329, 257-265.                                 | 5.4  | 198       |
| 4  | A comparison of two algorithms for warping of analytical signals. <i>Analytica Chimica Acta</i> , 2002, 456, 77-92.   | 5.4  | 195       |
| 5  | The Radial Basis Functions " Partial Least Squares approach as a flexible non-linear regression technique. <i>Analytica Chimica Acta</i> , 1996, 331, 177-185.  | 5.4  | 192       |
| 6  | TOMCAT: A MATLAB toolbox for multivariate calibration techniques. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2007, 85, 269-277.   | 3.5  | 170       |
| 7  | Raman spectroscopy as a process analytical technology (PAT) tool for the in-line monitoring and understanding of a powder blending process. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2008, 48, 772-779. | 2.8  | 132       |
| 8  | Tracing the geographical origin of honeys based on volatile compounds profiles assessment using pattern recognition techniques. <i>Food Chemistry</i> , 2010, 118, 171-176.   | 8.2  | 132       |
| 9  | Application of Wavelet Packet Transform in Pattern Recognition of Near-IR Data. <i>Analytical Chemistry</i> , 1996, 68, 1742-1747.  | 6.5  | 117       |
| 10 | Comparison of multivariate methods based on latent vectors and methods based on wavelength selection for the analysis of near-infrared spectroscopic data. <i>Analytica Chimica Acta</i> , 1995, 304, 285-295.            | 5.4  | 114       |
| 11 | Application of Wavelet Transform To Extract the Relevant Component from Spectral Data for Multivariate Calibration. <i>Analytical Chemistry</i> , 1997, 69, 4317-4323.  | 6.5  | 109       |
| 12 | Dealing with missing values and outliers in principal component analysis. <i>Talanta</i> , 2007, 72, 172-178.   | 5.5  | 105       |
| 13 | Chemometrics in analytical chemistry" part II: modeling, validation, and applications. <i>Analytical and Bioanalytical Chemistry</i> , 2018, 410, 6691-6704.  | 3.7  | 102       |
| 14 | Spectral transformation and wavelength selection in near-infrared spectra classification. <i>Analytica Chimica Acta</i> , 1995, 315, 243-255.   | 5.4  | 101       |
| 15 | Use and abuse of chemometrics in chromatography. <i>TrAC - Trends in Analytical Chemistry</i> , 2006, 25, 1081-1096.  | 11.4 | 101       |
| 16 | Chemometrics in analytical chemistry" part I: history, experimental design and data analysis tools. <i>Analytical and Bioanalytical Chemistry</i> , 2017, 409, 5891-5899.   | 3.7  | 95        |
| 17 | Fuzzy warping of chromatograms. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2005, 77, 173-180.   | 3.5  | 91        |
| 18 | Looking for Natural Patterns in Analytical Data. 2. Tracing Local Density with OPTICS. <i>Journal of Chemical Information and Computer Sciences</i> , 2002, 42, 500-507.  | 2.8  | 88        |

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|----|--|------|-----------|
| 19 | The comparative molecular surface analysis (COMSA): a novel tool for molecular design. <i>Computers &amp; Chemistry</i> , 2000, 24, 615-625.   | 1.2  | 87        |
| 20 | Wavelets " something for analytical chemistry?. <i>TrAC - Trends in Analytical Chemistry</i> , 1997, 16, 451-463.  | 11.4 | 86        |
| 21 | What can go wrong at the data normalization step for identification of biomarkers?. <i>Journal of Chromatography A</i> , 2014, 1362, 194-205.  | 3.7  | 86        |
| 22 | Comparison of Multivariate Calibration Techniques Applied to Experimental NIR Data Sets. <i>Applied Spectroscopy</i> , 2000, 54, 608-623.  | 2.2  | 81        |
| 23 | The Use of Wavelets for Signal Denoising in Capillary Electrophoresis. <i>Analytical Chemistry</i> , 2001, 73, 4903-4917.  | 6.5  | 75        |
| 24 | Application of Radial Basis Functions " Partial Least Squares to non-linear pattern recognition problems: diagnosis of process faults. <i>Analytica Chimica Acta</i> , 1996, 331, 187-193.   | 5.4  | 65        |
| 25 | Peak Alignment of Urine NMR Spectra Using Fuzzy Warping. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 863-875.  | 5.4  | 62        |
| 26 | Start-to-end processing of two-dimensional gel electrophoretic images. <i>Journal of Chromatography A</i> , 2007, 1158, 306-317.   | 3.7  | 60        |
| 27 | VSN: Variable sorting for normalization. <i>Journal of Chemometrics</i> , 2020, 34, e3164.   | 1.3  | 59        |
| 28 | Three-way principal component analysis applied to food analysis: an example. <i>Analytica Chimica Acta</i> , 2002, 462, 133-148.   | 5.4  | 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. <i>Talanta</i> , 2015, 134, 360-365. | 5.5  | 57        |
| 30 | A Comparison of Positive Matrix Factorization and the Weighted Multivariate Curve Resolution Method. Application to Environmental Data. <i>Environmental Science &amp; Technology</i> , 2011, 45, 10102-10110.                             | 10.0 | 56        |
| 31 | Robust partial least squares model for prediction of green tea antioxidant capacity from chromatograms. <i>Journal of Chromatography A</i> , 2007, 1176, 12-18.  | 3.7  | 53        |
| 32 | Preprocessing of two-dimensional gel electrophoresis images. <i>Proteomics</i> , 2004, 4, 2377-2389.   | 2.2  | 52        |
| 33 | About kernel latent variable approaches and SVM. <i>Journal of Chemometrics</i> , 2005, 19, 341-354.   | 1.3  | 51        |
| 34 | Target selection for alignment of chromatographic signals obtained using monochannel detectors. <i>Journal of Chromatography A</i> , 2007, 1176, 1-11.   | 3.7  | 51        |
| 35 | Near-infrared reflectance spectroscopy and multivariate calibration techniques applied to modelling the crude protein, fibre and fat content in rapeseed meal. <i>Analyst</i> , 2008, 133, 1523.   | 3.5  | 50        |
| 36 | Analysis of variance of designed chromatographic data sets: The analysis of variance-target projection approach. <i>Journal of Chromatography A</i> , 2015, 1405, 94-102.  | 3.7  | 46        |

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|----|--|------|-----------|
| 37 | Multiple factor analysis in environmental chemistry. <i>Analytica Chimica Acta</i> , 2005, 545, 1-12.  | 5.4  | 43        |
| 38 | Instrumentation of a roll compactor and the evaluation of the parameter settings by neural networks. <i>International Journal of Pharmaceutics</i> , 1997, 148, 103-115.                                   | 5.2  | 41        |
| 39 | Automated alignment of one-dimensional chromatographic fingerprints. <i>Journal of Chromatography A</i> , 2010, 1217, 6127-6133.   | 3.7  | 40        |
| 40 | Non-linear modelling of chemical data by combinations of linear and neural net methods. <i>Analytica Chimica Acta</i> , 1993, 283, 508-517.  | 5.4  | 38        |
| 41 | Pixel-based analysis of multiple images for the identification of changes: A novel approach applied to unravel proteome patterns of 2D electrophoresis gel images. <i>Proteomics</i> , 2007, 7, 3450-3461. | 2.2  | 38        |
| 42 | Classification and Regression Trees Studies of HIV Reverse Transcriptase Inhibitors. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 716-726.                                     | 2.8  | 37        |
| 43 | Transfer of Calibrations of Near-Infrared Spectra Using Neural Networks. <i>Applied Spectroscopy</i> , 1998, 52, 732-745.  | 2.2  | 36        |
| 44 | Factor analysis and experiment design in high-performance liquid chromatography. <i>Journal of Chromatography A</i> , 1987, 395, 183-202.  | 3.7  | 34        |
| 45 | Concept of (dis)similarity in data analysis. <i>TrAC - Trends in Analytical Chemistry</i> , 2012, 38, 116-128.   | 11.4 | 33        |
| 46 | Neural networks with robust backpropagation learning algorithm. <i>Analytica Chimica Acta</i> , 1996, 322, 21-29.  | 5.4  | 32        |
| 47 | Feature Based Fuzzy Matching of 2D Gel Electrophoresis Images. <i>Journal of Chemical Information and Computer Sciences</i> , 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. <i>Journal of Chemical Information and Computer Sciences</i> , 2002, 42, 1378-1389.                 | 2.8  | 32        |
| 49 | Proteomic analysis of striatal neuronal cell cultures after morphine administration. <i>Journal of Separation Science</i> , 2009, 32, 1200-1210.   | 2.5  | 31        |
| 50 | Calibration of somatic cell count in milk based on near-infrared spectroscopy. <i>Analytica Chimica Acta</i> , 2001, 450, 131-141.   | 5.4  | 29        |
| 51 | The Proteomic Analysis of Primary Cortical Astrocyte Cell Culture after Morphine Administration. <i>Journal of Proteome Research</i> , 2009, 8, 4633-4640.   | 3.7  | 28        |
| 52 | Maize proteomic responses to separate or overlapping soil drought and two-spotted spider mite stresses. <i>Planta</i> , 2016, 244, 939-960.  | 3.2  | 28        |
| 53 | Factor analysis and experiment design in high-performance liquid chromatography. <i>Journal of Chromatography A</i> , 1986, 353, 109-121.  | 3.7  | 27        |
| 54 | Factor analysis and experiment design in high-performance liquid chromatography. <i>Journal of Chromatography A</i> , 1986, 371, 253-267.  | 3.7  | 27        |

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|----|---|-----|-----------|
| 55 | A journey into low-dimensional spaces with autoassociative neural networks. <i>Talanta</i> , 2003, 59, 1095-1105.   | 5.5 | 27        |
| 56 | Factor analysis and experiment design in high-performance liquid chromatography. <i>Journal of Chromatography A</i> , 1986, 353, 123-137.   | 3.7 | 26        |
| 57 | Simultaneous optimisation of extraction of xanthone and benzophenone $\beta$ -glucosidase inhibitors from <i>Cyclopia genistoides</i> and identification of superior genotypes for propagation. <i>Journal of Functional Foods</i> , 2017, 33, 21-31. | 3.4 | 23        |
| 58 | Feature reduction by Fourier transform in pattern recognition of NIR data. <i>Analytica Chimica Acta</i> , 1996, 331, 75-83.  | 5.4 | 22        |
| 59 | Principal component analysis of dissolution data with missing elements. <i>International Journal of Pharmaceutics</i> , 2002, 234, 169-178.   | 5.2 | 21        |
| 60 | Modeling of the total antioxidant capacity of rooibos ( <i>Aspalathus linearis</i> ) tea infusions from chromatographic fingerprints and identification of potential antioxidant markers. <i>Journal of Chromatography A</i> , 2014, 1366, 101-109.   | 3.7 | 21        |
| 61 | How to construct a multiple regression model for data with missing elements and outlying objects. <i>Analytica Chimica Acta</i> , 2007, 581, 324-332.   | 5.4 | 20        |
| 62 | Matching 2D Gel Electrophoresis Images. <i>Journal of Chemical Information and Computer Sciences</i> , 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. <i>Food Research International</i> , 2019, 121, 185-196.                                       | 6.2 | 18        |
| 64 | A neuro-fuzzy system for X-ray spectra interpretation. <i>Mikrochimica Acta</i> , 1994, 113, 153-169.   | 5.0 | 17        |
| 65 | Discrimination of biofilm samples using pattern recognition techniques. <i>Analytical and Bioanalytical Chemistry</i> , 2008, 390, 1273-1282.   | 3.7 | 17        |
| 66 | Relating gas chromatographic profiles to sensory measurements describing the end products of the Maillard reaction. <i>Talanta</i> , 2011, 83, 1239-1246.   | 5.5 | 17        |
| 67 | Classification of data with missing elements and outliers. <i>Talanta</i> , 2008, 76, 602-609.  | 5.5 | 16        |
| 68 | Robust biomarker identification in a two-class problem based on pairwise log-ratios. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2017, 171, 277-285.   | 3.5 | 16        |
| 69 | Again about partial least squares and feature selection. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2012, 115, 9-17.  | 3.5 | 15        |
| 70 | Classification of genomic data: Some aspects of feature selection. <i>Talanta</i> , 2008, 76, 564-574.  | 5.5 | 13        |
| 71 | Multivariate analysis of variance of designed chromatographic data. A case study involving fermentation of rooibos tea. <i>Journal of Chromatography A</i> , 2017, 1489, 115-125.   | 3.7 | 13        |
| 72 | Different strategies for class model optimization. A comparative study. <i>Talanta</i> , 2020, 215, 120912.   | 5.5 | 12        |

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|----|--|-----|-----------|
| 73 | Genotypic variation in phenolic composition of <i>Cyclopia pubescens</i> (honeybush tea) seedling plants. <i>Journal of Food Composition and Analysis</i> , 2019, 78, 129-137.   | 3.9 | 11        |
| 74 | Authentication of honeybush and rooibos herbal teas based on their elemental composition. <i>Food Control</i> , 2021, 123, 107757.   | 5.5 | 9         |
| 75 | High-temperature oxidation reduces the bitterness of honeybush infusions depending on changes in phenolic composition. <i>LWT - Food Science and Technology</i> , 2021, 139, 110608.   | 5.2 | 9         |
| 76 | Non-parametric multivariate analysis of variance in the proteomic response of potato to drought stress. <i>Analytica Chimica Acta</i> , 2012, 719, 1-7.  | 5.4 | 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. <i>Spectrochimica Acta, Part B: Atomic Spectroscopy</i> , 2021, 177, 106069. | 2.9 | 8         |
| 78 | Cellulose sorbents in investigations on self-association of higher fatty alcohols. <i>Microchemical Journal</i> , 1981, 26, 299-306.   | 4.5 | 7         |
| 79 | Robust Methods in Analysis of Multivariate Food Chemistry Data. <i>Data Handling in Science and Technology</i> , 2013, , 315-340.  | 3.1 | 7         |
| 80 | Model development for predicting <i>in vitro</i> bio-capacity of green rooibos extract based on composition for application as screening tool in quality control. <i>Food and Function</i> , 2020, 11, 3084-3094.  | 4.6 | 7         |
| 81 | Class-modelling of overlapping classes. A two-step authentication approach. <i>Analytica Chimica Acta</i> , 2022, 1191, 339284.  | 5.4 | 7         |
| 82 | Combining class-modelling and discriminant methods for improvement of products authentication. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2022, 228, 104620.   | 3.5 | 7         |
| 83 | Finding relevant clustering directions in high-dimensional data using Particle Swarm Optimization. <i>Journal of Chemometrics</i> , 2011, 25, 366-374.   | 1.3 | 6         |
| 84 | SEPARATION OF CHALCONES ISOMERS IN HPLC SYSTEMS. <i>Analytical Sciences</i> , 1991, 7, 103-107.  | 1.6 | 5         |
| 85 | The scope of applicability of the selected class-modelling methods. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2021, 218, 104427.  | 3.5 | 5         |
| 86 | Working with log-ratios. <i>Analytica Chimica Acta</i> , 2019, 1059, 16-27.  | 5.4 | 4         |
| 87 | Chromatographic and spectroscopic investigation of the associative changes with the selected higher fatty alcohols. <i>Microchemical Journal</i> , 1980, 25, 330-337.  | 4.5 | 3         |
| 88 | Wavelet Bases for IR Library Compression, Searching and Reconstruction. <i>Data Handling in Science and Technology</i> , 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. <i>Journal of Food Composition and Analysis</i> , 2021, 102, 104041.  | 3.9 | 3         |

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|-----|--|------|-----------|
| 91  | European analytical column. TrAC - Trends in Analytical Chemistry, 2014, 56, ix-xii.   | 11.4 | 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. | 3.7  | 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.                                  | 4.5  | 0         |
| 95  | Estimation of the number of true null hypotheses when conducting a multiple testing. Chemometrics and Intelligent Laboratory Systems, 2010, 104, 281-288.        | 3.5  | 0         |
| 96  | A new concept for variance analysis of hyphenated chromatographic data avoiding signal warping. Journal of Chromatography A, 2013, 1291, 64-72.                  | 3.7  | 0         |
| 97  | European Analytical Column Number 42. Journal of Analytical Chemistry, 2014, 69, 812-816.  | 0.9  | 0         |
| 98  | European analytical column number 42. Accreditation and Quality Assurance, 2014, 19, 225-229.  | 0.8  | 0         |
| 99  | Particle Swarm Optimization. , 2020, , 649-666.  |      | 0         |
| 100 | Chemometria w metabolomice i proteomice. , 2010, , .   |      | 0         |