Partial least squares discriminant analysis: taking the magic away

#	Paper	IF	Citations
498	WITHDRAWN: Recent advances in chemometric methods for plant metabolomics: A review. **2014**,		3
497	A comparison of different chemometrics approaches for the robust classification of electronic nose data. **2014**, 406, 7581-90		50
496	Influence of missing values substitutes on multivariate analysis of metabolomics data. **2014**, 4, 433-52		115
495	Method for identification of spectral targets in discrete frequency infrared spectroscopy for clinical diagnostics. **2015**, 69, 1066-73		14
494	Swarm Intelligence for Chemometrics. **2015**, 26, 7-11		2
493	A tutorial review: Metabolomics and partial least squares-discriminant analysis--a marriage of convenience or a shotgun wedding. **2015**, 879, 10-23		478
492	Evaluation of supervised chemometric methods for sample classification by Laser Induced Breakdown Spectroscopy. **2015**, 146, 354-364		54
491	Chemometrics and qualitative analysis have a vibrant relationship. **2015**, 69, 34-51		68
490	Detection of discoloration in diesel fuel based on gas chromatographic fingerprints. **2015**, 407, 1159-70		18
489	Pursuing shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS) for concomitant detection of breast lesions and microcalcifications. **2015**, 7, 16960-8		33
488	Hierarchical Classification Modeling of Watershed Data by Chemical Signatures. **2015**, 159-193		2
487	Fusion of the H NMR data of serum, urine and exhaled breath condensate in order to discriminate chronic obstructive pulmonary disease and obstructive sleep apnea syndrome. **2015**, 11, 1563-1574		26
486	Pattern recognition in chemometrics. **2015**, 149, 90-96		78
485	Simple and Effective Way for Data Preprocessing Selection Based on Design of Experiments. *Analytical Chemistry*, **2015**, 87, 12096-103	7.8	92
484	Metabolomics with Nuclear Magnetic Resonance Spectroscopy in a Drosophila melanogaster Model of Surviving Sepsis. **2016**, 6,		11
483	Material properties of Islamic paper. **2016**, 4,		8
482	A profile of volatile organic compounds in exhaled air as a potential non-invasive biomarker for liver cirrhosis. **2016**, 6, 19903		36

481 Rapid Identification of Biotherapeutics with Label-Free Raman Spectroscopy. *Analytical Chemistry*, **2016**, 88, 4361-8 — 7.8 — 24

480 Determining the geographical origin of Sechium edule fruits by multielement analysis and advanced chemometric techniques. **2016**, 210, 228-34 — 19

479 Non-targeted metabolite profiling reveals changes in oxidative stress, tryptophan and lipid metabolisms in fearful dogs. **2016**, 12, 7 — 21

478 Detection and characterisation of frauds in bovine meat in natura by non-meat ingredient additions using data fusion of chemical parameters and ATR-FTIR spectroscopy. **2016**, 205, 14-22 — 67

477 Chemometrics and the identification of counterfeit medicines-A review. **2016**, 127, 112-22 — 26

476 Point-of-use electroanalytical platform based on homemade potentiostat and smartphone for multivariate data processing. **2016**, 219, 170-177 — 31

475 Differences in microbial metabolites in urine headspace of subjects with Immune Thrombocytopenia (ITP) detected by volatile organic compound (VOC) analysis and metabolomics. *Clinica Chimica Acta*, **2016**, 461, 61-8 — 6.2 — 5

474 Identification and discrimination of three common Aloe species by high performance liquid chromatography-tandem mass spectrometry coupled with multivariate analysis. **2016**, 1031, 163-171 — 10

473 Challenges of large-class-number classification (LCNC): A novel ensemble strategy (ES) and its application to discriminating the geographical origins of 25 green teas. **2016**, 157, 43-49 — 15

472 Statistical Health Monitoring Applied to a Metabolomic Study of Experimental Hepatocarcinogenesis: An Alternative Approach to Supervised Methods for the Identification of False Positives. *Analytical Chemistry*, **2016**, 88, 7921-9 — 7.8 — 6

471 Strategy of integrated evaluation on treatment of traditional Chinese medicine as 'interaction of system to system' and establishment of novel fuzzy target contribution recognition with herb-pairs, a case study on Astragali Radix-Fructus Corni. **2016**, 434, 219-37 — 7

470 Mass spectrometry for the characterization of brewing process. *Food Research International*, **2016**, 89, 281-288 — 7 — 8

469 The successive projections algorithm for interval selection in partial least squares discriminant analysis. **2016**, 8, 7522-7530 — 6

468 Networkmetrics: multivariate big data analysis in the context of the internet. *Journal of Chemometrics*, **2016**, 30, 488-505 — 1.6 — 8

467 Serum metabolomics profiles in response to n-3 fatty acids in Chinese patients with type 2 diabetes: a double-blind randomised controlled trial. **2016**, 6, 29522 — 22

466 Vocabulary of concepts and terms in chemometrics (IUPAC Recommendations 2016). **2016**, 88, 407-443 — 38

465 LC-MS based global metabolite profiling: the necessity of high data quality. **2016**, 12, 1 — 34

464 Variable selection for binary classification using error rate p-values applied to metabolomics data. **2016**, 17, 33 — 4

463	Comparison of classification methods with İ-classİreceiver operating characteristic curves: A case study of energy drinks. **2016**, 151, 34-43		11
462	Nondestructive Total Excitation-Emission Fluorescence Microscopy Combined with Multi-Way Chemometric Analysis for Visually Indistinguishable Single Fiber Discrimination. *Analytical Chemistry*, **2016**, 88, 2967-75	7.8	18
461	The Monte Carlo validation framework for the discriminant partial least squares model extended with variable selection methods applied to authenticity studies of Viagra based on chromatographic impurity profiles. **2016**, 141, 1060-70		22
460	Multivariate data analysis and metabolic profiling of artemisinin and related compounds in high yielding varieties of Artemisia annua field-grown in Madagascar. **2016**, 117, 522-31		16
459	Differentiation between two "fang ji" herbal medicines, Stephania tetrandra and the nephrotoxic Aristolochia fangchi, using hyperspectral imaging. **2016**, 122, 213-222		30
458	Differential gene expression in human, murine, and cell line-derived macrophages upon polarization. **2016**, 347, 1-13		94
457	A potential tool for diagnosis of male infertility: Plasma metabolomics based on GC-MS. **2016**, 147, 82-9		34
456	A Chemometrics Approach to the Investigation of the Intraspecific Variability of the Volatile Oil of Eupatorium tremulum from Southern Brazil. **2017**, 80, 45-52		6
455	Systems serology for evaluation of HIV vaccine trials. **2017**, 275, 262-270		47
454	Stress-sensitive arterial hypertension, haemodynamic changes and brain metabolites in hypertensive ISIAH rats: MRI investigation. **2017**, 102, 523-532		14
453	A contemporary review on Data Preprocessing (DP) practice strategy in ATR-FTIR spectrum. **2017**, 163, 64-75		72
452	Discrimination of whisky brands and counterfeit identification by UV-Vis spectroscopy and multivariate data analysis. **2017**, 229, 142-151		69
451	Inventory and Assessment of thePan troglodytes(Blumenbach, 1799) Skeletal Collection Housed at the Yale Peabody Museum. **2017**, 58, 209-259		2
450	Systematic examination of the incorporation of class relationships via multilabel, multiclass, hierarchical classification. *Journal of Chemometrics*, **2017**, 31, e2885	1.6	3
449	Evaluation and identification of blood stains with handheld NIR spectrometer. *Microchemical Journal*, **2017**, 133, 561-566	4.8	33
448	Comparison of multivariate classification algorithms using EEM fluorescence data to distinguish Cryptococcus neoformans and Cryptococcus gattii pathogenic fungi. **2017**, 9, 3968-3976		6
447	Variation analysis in spectral indices of volatile chlorpyrifos and non-volatile imidacloprid in jujube (Ziziphus jujuba Mill.) using near-infrared hyperspectral imaging (NIR-HSI) and gas chromatograph-mass spectrometry (GCMS). **2017**, 139, 41-55		32
446	Geochemical Fingerprinting by Handheld Laser-Induced Breakdown Spectroscopy. **2017**, 41, 563-584		41

445	Class-modelling in food analytical chemistry: Development, sampling, optimisation and validation issues - A tutorial. **2017**, 982, 9-19		112
444	Forensic discrimination between authentic and counterfeit perfumes using paper spray mass spectrometry and multivariate supervised classification. **2017**, 9, 4979-4987		12
443	Mass spectrometry based metabolomics for in vitro systems pharmacology: pitfalls, challenges, and computational solutions. **2017**, 13, 79		19
442	Paper spray mass spectrometry and chemometric tools for a fast and reliable identification of counterfeit blended Scottish whiskies. **2017**, 237, 1058-1064		30
441	Chemical profiling of floral and chestnut honey using high-performance liquid chromatography-ultraviolet detection. **2017**, 62, 205-210		7
440	Screening of Wolbachia Endosymbiont Infection in Aedes aegypti Mosquitoes Using Attenuated Total Reflection Mid-Infrared Spectroscopy. *Analytical Chemistry*, **2017**, 89, 5285-5293	7.8	18
439	Direct classification of new psychoactive substances in seized blotter papers by ATR-FTIR and multivariate discriminant analysis. *Microchemical Journal*, **2017**, 133, 96-103	4.8	15
438	Stable biomarker screening and classification by subsampling-based sparse regularization coupled with support vector machines in metabolomics. **2017**, 160, 22-31		17
437	A high-order representation and classification method for transcription factor binding sites recognition in Escherichia coli. **2017**, 75, 16-23		2
436	Discriminating Lacustrine and Marine Organic Matter Depositional Paleoenvironments of Brazilian Crude Oils Using Comprehensive Two-Dimensional Gas Chromatography Quadrupole Mass Spectrometry and Supervised Classification Chemometric Approaches. **2017**, 31, 170-178		8
435	NMR-based metabolomics strategies: plants, animals and humans. **2017**, 9, 1078-1096		43
434	Geochemistry of magnetite and hematite from unmineralized bedrock and local till at the Kiggavik uranium deposit: Implications for sediment provenance. **2017**, 183, 1-21		12
433	Spectroscopy with computational analysis in virological studies: A decade (2006-2016). **2017**, 97, 244-256		35
432	Recent chemometrics advances for foodomics. **2017**, 96, 42-51		61
431	Chemometrics for Food Quality Control and Authentication. **2017**, 1-29		3
430	Spectral Mining for Discriminating Blood Origins in the Presence of Substrate Interference via Attenuated Total Reflection Fourier Transform Infrared Spectroscopy: Postmortem or Antemortem Blood?. *Analytical Chemistry*, **2017**, 89, 9797-9804	7.8	13
429	Optimal preprocessing of serum and urine metabolomic data fusion for staging prostate cancer through design of experiment. **2017**, 991, 68-75		20
428	Detecting semen stains on fabrics using near infrared hyperspectral images and multivariate models. **2017**, 95, 23-35		25

| 427 | Differentiation of hair using ATR FT-IR spectroscopy: A statistical classification of dyed and non-dyed hairs. *Forensic Chemistry*, **2017**, 6, 1-9 | 2.8 | 22 |

| 426 | Toward a Noninvasive, Label-Free Screening Method for Determining Spore Inoculum Quality of Penicillium chrysogenum Using Raman Spectroscopy. **2017**, 71, 2661-2669 | | 3 |

| 425 | Model-Based Methods in the Biopharmaceutical Process Lifecycle. **2017**, 34, 2596-2613 | | 45 |

| 424 | Rapid and sensitive method for determining free amino acids in plant tissue by high-performance liquid chromatography with fluorescence detection. **2017**, 36, 680-696 | | 8 |

| 423 | Latent Variable Regression for Laboratory Hyperspectral Images. **2017**, 339-365 | | 1 |

| 422 | Exploring Morphological and Biochemical Linkages in Fungal Growth with Label-Free Light Sheet Microscopy and Raman Spectroscopy. **2017**, 18, 72-78 | | 24 |

| 421 | Plasma sample based analysis of gastric cancer progression using targeted metabolomics. **2017**, 7, 17774 | | 33 |

| 420 | Evaluation of Classifier Performance for Multiclass Phenotype Discrimination in Untargeted Metabolomics. **2017**, 7, | | 23 |

| 419 | Outlier Detection in Dynamic Systems with Multiple Operating Points and Application to Improve Industrial Flare Monitoring. **2017**, 5, 28 | | 4 |

| 418 | Determination of the country of origin of true mahogany (Swietenia macrophylla King) wood in five Latin American countries using handheld NIR devices and multivariate data analysis. **2018**, 72, 521-530 | | 16 |

| 417 | Multivariate Analysis of Multiple Datasets: a Practical Guide for Chemical Ecology. **2018**, 44, 215-234 | | 44 |

| 416 | Raman spectroscopy coupled to chemometrics to discriminate provenance and geological age of amber. **2018**, 49, 842-851 | | 11 |

| 415 | Evaluation and classification of eucalypt charcoal quality by near infrared spectroscopy. **2018**, 112, 85-92 | | 18 |

| 414 | Evidence that the metabolite repair enzyme NAD(P)HX epimerase has a moonlighting function. **2018**, 38, | | 12 |

| 413 | Multiclass partial least squares discriminant analysis: Taking the right way—A critical tutorial. *Journal of Chemometrics*, **2018**, 32, e3030 | 1.6 | 15 |

| 412 | Metabolomic response to coffee consumption: application to a three-stage clinical trial. **2018**, 283, 544-557 | | 30 |

| 411 | Simultaneous quantification of caffeine and chlorogenic acid in coffee green beans and varietal classification of the samples by HPLC-DAD coupled with chemometrics. *Environmental Science and Pollution Research*, **2018**, 25, 28748-28759 | 5.1 | 26 |

| 410 | Mid-IR hyperspectral imaging for label-free histopathology and cytology. **2018**, 20, 023002 | | 44 |

409	Significance of variables for discrimination: Applied to the search of organic ions in mass spectra measured on cometary particles. *Journal of Chemometrics*, **2018**, 32, e3001	1.6	1
408	The quantification of free Amadori compounds and amino acids allows to model the bound Maillard reaction products formation in soybean products. **2018**, 247, 29-38		20
407	Incremental feature extraction based on decision boundaries. **2018**, 77, 65-74		10
406	In vivo study of dermal collagen of striae distensae by confocal Raman spectroscopy. **2018**, 33, 609-617		4
405	Infrared spectroscopy and multivariate methods as a tool for identification and quantification of fuels and lubricant oils in soil. **2018**, 190, 72		8
404	Systems biology as an emerging paradigm in transfusion medicine. **2018**, 12, 31		8
403	Simultaneous detection of multiple inherited metabolic diseases using GC-MS urinary metabolomics by chemometrics multi-class classification strategies. **2018**, 186, 489-496		13
402	Predicting ionic liquid melting points using machine learning. **2018**, 264, 318-326		38
401	Statistical processing of compositional data. The case of ceramic samples from the archaeological site of Xalasco, Tlaxcala, Mexico. **2018**, 19, 100-114		4
400	Evaluation of attached mortar on recycled concrete aggregates by hyperspectral imaging. **2018**, 169, 835-842		28
399	Consensus Classification Using Non-Optimized Classifiers. *Analytical Chemistry*, **2018**, 90, 4429-4437	7.8	14
398	Aluminium foil as an alternative substrate for the spectroscopic interrogation of endometrial cancer. **2018**, 11, e201700372		10
397	Autofluorescence imaging identifies tumor cell-cycle status on a single-cell level. **2018**, 11, e201600276		21
396	Detection and quantification of extra virgin olive oil adulteration by means of autofluorescence excitation-emission profiles combined with multi-way classification. **2018**, 178, 751-762		50
395	A review of algorithms for SAW sensors e-nose based volatile compound identification. *Sensors and Actuators B: Chemical*, **2018**, 255, 2472-2482	8.5	29
394	Rapid and sensitive method for detecting adulterants in gasoline using ultra-fast gas chromatography and Partial Least Square Discriminant Analysis. **2018**, 215, 204-211		11
393	Fourier Transform Infrared and Raman and Hyperspectral Imaging Techniques for Quality Determinations of Powdery Foods: A Review. **2018**, 17, 104-122		84
392	MALDI-TOF-MS with PLS Modeling Enables Strain Typing of the Bacterial Plant Pathogen Xanthomonas axonopodis. **2018**, 29, 413-421		8

391	Critical review of reporting of the data analysis step in metabolomics. **2017**, 14, 7		37
390	Prospects from systems serology research. **2018**, 153, 279-289		38
389	Differentiation of cumin seeds using a metal-oxide based gas sensor array in tandem with chemometric tools. **2018**, 176, 221-226		17
388	A modified locality preserving partial least squares for classification problems. **2018**,		
387	Partial least squares discriminant analysis for chemometrics and metabolomics: How scores, loadings, and weights differ according to two common algorithms. *Journal of Chemometrics*, **2018**, 32, e3028	1.6	10
386	Multivariate Classification Techniques. **2018**,		3
385	A high-throughput serum Raman spectroscopy platform and methodology for colorectal cancer diagnostics. **2018**, 143, 6014-6024		30
384	Chemometrical and molecular methods in olive oil analysis: A review. **2018**, 42, e13770		9
383	Raman spectroscopic detection of high-grade cervical cytology: Using morphologically normal appearing cells. **2018**, 8, 15048		19
382	Integrated Chemometrics and Statistics to Drive Successful Proteomics Biomarker Discovery. **2018**, 6,		13
381	Variable selection in omics data: A practical evaluation of small sample sizes. **2018**, 13, e0197910		25
380	Fearful dogs have increased plasma glutamine and Eglutamyl glutamine. **2018**, 8, 15976		10
379	Effects of data pre-processing methods on classification of ATR-FTIR spectra of pen inks using partial least squares-discriminant analysis (PLS-DA). **2018**, 182, 90-100		13
378	Discriminating volcanic centers with handheld laser-induced breakdown spectroscopy (LIBS). *Journal of Archaeological Science*, **2018**, 98, 112-127	2.9	25
377	Intracellular amino and nonamino organic acids profiling of Trichosporon cutaneum on rich and limited nitrogen conditions for lipid production. **2018**, 118, 84-92		1
376	Metabolomics approach in lung tissue of septic rats and the interventional effects of Xuebijing injection using UHPLC-Q-Orbitrap-HRMS. **2018**, 164, 427-435		7
375	Development and comparison of regression models for the determination of quality parameters in margarine spread samples using NIR spectroscopy. **2018**, 10, 3089-3099		5
374	Implications of measurement error structure on the visualization of multivariate chemical data: hazards and alternatives. **2018**, 96, 738-748		6

373	Designing Algorithms To Aid Discovery by Chemical Robots. **2018**, 4, 793-804		45
372	Overoptimism in cross-validation when using partial least squares-discriminant analysis for omics data: a systematic study. **2018**, 410, 5981-5992		27
371	Novel Biomarker Candidates for Febrile Neutropenia in Hematological Patients Using Nontargeted Metabolomics. **2018**, 2018, 6964529		3
370	A mathematical model of in vivo bovine blastocyst developmental to gestational Day 15. **2018**, 101, 8401-8416		1
369	Analysis of gas sensors array signals for evaluation of mold contamination in buildings. **2018**,		1
368	Modeling second-order data for classification issues: Data characteristics, algorithms, processing procedures and applications. **2018**, 107, 151-168		22
367	Image-based manufacturing analytics: Improving the accuracy of an industrial pellet classification system using deep neural networks. **2018**, 180, 26-35		11
366	Comprehensive Two-Dimensional Gas Chromatography Mass Spectrometry/Selected Ion Monitoring (GC GC MS/SIM) and Chemometrics to Enhance Inter-Reservoir Geochemical Features of Crude Oils. **2018**, 32, 8017-8023		6
365	Application of Image Texture Analysis for Evaluation of X-Ray Images of Fungal-Infected Maize Kernels. **2018**, 11, 2799-2815		2
364	Stereoselective accumulations of hexachlorocyclohexanes (HCHs) are correlated with Sphingomonas spp. in agricultural soils across China. **2018**, 240, 27-33		16
363	Apigenin inhibits growth of the Plasmodium berghei and disrupts some metabolic pathways in mice. **2018**, 32, 1795-1802		8
362	Screening method for rapid classification of psychoactive substances in illicit tablets using mid infrared spectroscopy and PLS-DA. *Forensic Science International*, **2018**, 288, 227-235	2.6	23
361	Variable selection for multivariate classification aiming to detect individual adulterants and their blends in grape nectars. **2018**, 190, 55-61		18
360	Biomarkers of Physiological Responses to Periods of Intensified, Non-Resistance-Based Exercise Training in Well-Trained Male Athletes: A Systematic Review and Meta-Analysis. **2018**, 48, 2517-2548		32
359	Collaborative representation based classifier with partial least squares regression for the classification of spectral data. **2018**, 182, 79-86		5
358	Compositional Data Analysis with PLS-DA and Security Applications. **2018**,		3
357	Partial least squares-discriminant analysis (PLS-DA) for classification of high-dimensional (HD) data: a review of contemporary practice strategies and knowledge gaps. **2018**, 143, 3526-3539		219
356	On the utilization of principal component analysis in laser-induced breakdown spectroscopy data analysis, a review. **2018**, 148, 65-82		93

355	Potential of mid-infrared spectroscopy as a non-invasive diagnostic test in urine for endometrial or ovarian cancer. **2018**, 143, 3156-3163		32
354	UPLC-Orbitrap-MS/MS combined with chemometrics establishes variations in chemical components in green tea from Yunnan and Hunan origins. **2018**, 266, 534-544		50
353	Predictive metabolomic signatures of end-stage renal disease: A multivariate analysis of population-based data. **2018**, 152, 14-30		14
352	Classification of cowpea beans using multielemental fingerprinting combined with supervised learning. **2019**, 95, 232-241		7
351	Trace element composition of iron oxides from IOCG and IOA deposits: relationship to hydrothermal alteration and deposit subtypes. *Mineralium Deposita*, **2019**, 54, 525-552	4.8	41
350	Mass Spectrometry-Based Metabolomic Analysis. **2019**, 410-425		1
349	Identification of NBOMe and NBOH in blotter papers using a handheld NIR spectrometer and chemometric methods. *Microchemical Journal*, **2019**, 144, 151-158	4.8	15
348	Multivariate Calibration. **2019**, 87-129		
347	Potential biomonitoring of atmospheric carbon dioxide in Coffea arabica leaves using near-infrared spectroscopy and partial least squares discriminant analysis. *Environmental Science and Pollution Research*, **2019**, 26, 30356-30364	5.1	9
346	Detecting chemical markers to uncover counterfeit rebated excise duty diesel oil. **2019**, 204, 229-237		3
345	The effects of different land use patterns on the microclimate and ecosystem services in the agro-pastoral ecotone of Northern China. **2019**, 106, 105522		11
344	Multidimensional scaling assisted Fourier-transform infrared spectroscopic analysis of fruit wine samples: introducing a novel analytical approach. **2019**, 11, 4106-4115		1
343	Development of the Self Optimising Kohonen Index Network (SKiNET) for Raman Spectroscopy Based Detection of Anatomical Eye Tissue. **2019**, 9, 10812		13
342	Trace Element Composition of Igneous and Hydrothermal Magnetite from Porphyry Deposits: Relationship to Deposit Subtypes and Magmatic Affinity. **2019**, 114, 917-952		25
341	The Search for Clinically Useful Biomarkers of Complex Disease: A Data Analysis Perspective. **2019**, 9,		17
340	Monitoring Radiotherapeutic Response in Prostate Cancer Patients Using High Throughput FTIR Spectroscopy of Liquid Biopsies. **2019**, 11,		11
339	Nonconvulsive epileptic seizure monitoring with incremental learning. **2019**, 114, 103434		2
338	Predictors of fatal outcomes in pedestrian accidents in Tabriz Metropolis of Iran: Application of PLS-DA method. **2019**, 20, 873-879		5

337 Tracing the dune activation of Badain Jaran Desert and Tengger Desert by using near infrared spectroscopy and chemometrics. **2019**, 27, 370-378 — 1

336 Identification of Luminescent Markers for Gunshot Residues: Fluorescence, Raman Spectroscopy, and Chemometrics. *Analytical Chemistry*, **2019**, 91, 12444-12452 — 7.8 — 14

335 Application of likelihood ratios and optimal decision thresholds in fire debris analysis based on a partial least squares discriminant analysis (PLS-DA) model. *Forensic Chemistry*, **2019**, 16, 100188 — 2.8 — 13

334 Avoiding nonsense in electronic taste sensing. **2019**, 121, 115675 — 8

333 Ranking strategies to support toxicity prediction: A case study on potential LXR binders. **2019**, 10, 130-144 — 1

332 Mass spectrometry-based metabolomic discrimination of Cercospora leaf spot resistant and susceptible sugar beet germplasms. **2019**, 215, 1 — 2

331 Disease-specific protein corona sensor arrays may have disease detection capacity. **2019**, 4, 1063-1076 — 41

330 Raman hyperspectral imaging and a novel approach for objective determination of the order of crossing ink lines. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 223, 117287 — 4.4 — 3

329 Analysis of Scotch Whisky by H NMR and chemometrics yields insight into its complex chemistry. **2019**, 298, 125052 — 14

328 Classification of commercial charcoal for domestic use by near infrared spectroscopy. **2019**, 127, 105280 — 2

327 Development of a methodology to analyze leaves from Prunus dulcis varieties using near infrared spectroscopy. **2019**, 204, 320-328 — 9

326 Predicting the absence of an unknown compound in a mass spectral database. **2019**, 25, 439-444 — 2

325 Improving data splitting for classification applications in spectrochemical analyses employing a random-mutation Kennard-Stone algorithm approach. **2019**, 35, 5257-5263 — 39

324 Plasma Sphingolipids Mediate a Relationship Between Type 2 Diabetes and Memory Outcomes in Patients with Coronary Artery Disease Undertaking Exercise. **2019**, 69, 717-727 — 4

323 Metabolomics: Experimental Design, Methodology, and Data Analysis. **2019**, 1-22

322 Application of Electronic Nose for Evaluation of Wastewater Treatment Process Effects at Full-Scale WWTP. **2019**, 7, 251 — 15

321 Ripeness Classification of Bananito Fruit (Musa acuminata, AA): a Comparison Study of Visible Spectroscopy and Hyperspectral Imaging. **2019**, 12, 1693-1704 — 19

320 A non-targeted LC-HRMS approach for detecting exposure to illegal veterinary treatments: The case of cephalosporins in commercial laying Hens. **2019**, 1599, 161-171 — 6

319	Spatiotemporal Variation Characteristics of Ecosystem Service Losses in the Agro-Pastoral Ecotone of Northern China. **2019**, 16,		7
318	An Integrated Approach to Plant Biology via Multi-Analogous Methods. **2019**, 57-126		
317	Instrumentation Applied to Metabolomic Analysis. **2019**, 239-292		
316	A deep learning- and partial least square regression-based model observer for a low-contrast lesion detection task in CT. **2019**, 46, 2052-2063		20
315	Alternative data mining/machine learning methods for the analytical evaluation of food quality and authenticity - A review. *Food Research International*, **2019**, 122, 25-39	7	107
314	Raman spectroscopy and discriminant analysis applied to the detection of frauds in bovine meat by the addition of salts and carrageenan. *Microchemical Journal*, **2019**, 147, 582-589	4.8	13
313	An ensemble variable selection method for vibrational spectroscopic data analysis.. **2019**, 9, 6708-6716		2
312	Predictive modelling of colossal ATR-FTIR spectral data using PLS-DA: empirical differences between PLS1-DA and PLS2-DA algorithms. **2019**, 144, 2670-2678		12
311	Ecological Metabolomics: Challenges and Perspectives. **2019**, 293-378		
310	"-Omics" workflow for paleolimnological and geological archives: A review. **2019**, 672, 438-455		10
309	TTWD-DA: A MATLAB toolbox for discriminant analysis based on trilinear three-way data. **2019**, 188, 46-53		10
308	Application of differential mobility-mass spectrometry for untargeted human plasma metabolomic analysis. **2019**, 411, 6297-6308		10
307	Data analytics on raw material properties to accelerate pharmaceutical drug development. *International Journal of Pharmaceutics*, **2019**, 563, 122-134	6.5	8
306	Standardization of complex biologically derived spectrochemical datasets. **2019**, 14, 1546-1577		61
305	Classification of six herbal bioactive compositions employing LAPV and PLS-DA. *Journal of Chemometrics*, **2019**, 33, e3112	1.6	4
304	Identification of a metabolomic signature associated with feed efficiency in beef cattle. **2019**, 20, 8		31
303	Amino Acid Biosignature in Plasma among Ischemic Stroke Subtypes. **2019**, 2019, 8480468		10
302	Developing infrared spectroscopic detection for stratifying brain tumour patients: glioblastoma multiforme vs. lymphoma. **2019**, 144, 6736-6750		21

301	Locality preserving partial least squares discriminant analysis for face recognition. **2019**,		4
300	Chlorophyll a fluorescence analysis can detect phosphorus deficiency under field conditions and is an effective tool to prevent grain yield reductions in spring barley (Hordeum vulgare L.). **2019**, 434, 79-91		23
299	Discrimination and classification of extra virgin olive oil using a chemometric approach based on TMS-4,4'-desmetylsterols GC(FID) fingerprints of edible vegetable oils. **2019**, 274, 518-525		13
298	Statistical analysis of proteomics data: A review on feature selection. **2019**, 198, 18-26		36
297	Data Analysis. **2019**, 81-94		1
296	Brain dynamics and temporal trajectories during task and naturalistic processing. **2019**, 186, 410-423		9
295	Machine learning combined with non-targeted LC-HRMS analysis for a risk warning system of chemical hazards in drinking water: A proof of concept. **2019**, 195, 426-432		20
294	Classification of pre-dyed textile fibers exposed to weathering and photodegradation by non-destructive excitation-emission fluorescence spectroscopy paired with discriminant unfolded-partial least squares. *Forensic Chemistry*, **2019**, 12, 25-32	2.8	6
293	The feasibility of applying NIR and FT-IR fingerprinting to detect adulteration in black pepper. **2019**, 100, 1-7		55
292	The potential of biobanked liquid based cytology samples for cervical cancer screening using Raman spectroscopy. **2019**, 12, e201800377		11
291	Effects of elevated CO concentration on leaves and berries of black elder (Sambucus nigra) using UHPLC-ESI-QTOF-MS/MS and gas exchange measurements. **2019**, 234-235, 71-79		6
290	Raw material quality assessment approaches comparison in pectin production. **2019**, 35, e2762		4
289	Comparison of flavonoid and policosanol profiles in Korean winter-spinach (Spinacia oleracea L.) cultivated in different regions. **2019**, 279, 202-208		12
288	Wine authentication: a fingerprinting multiclass strategy to classify red varietals through profound chemometric analysis of volatiles. **2019**, 245, 179-190		7
287	Statistical comparison of decision rules in PLS2-DA prediction model for classification of blue gel pen inks according to pen brand and pen model. **2019**, 184, 94-101		4
286	Matching service failures and recovery options toward satisfaction. **2019**, 39, 901-924		12
285	Comparison of Different Multivariate Classification Methods for the Detection of Adulterations in Grape Nectars by Using Low-Field Nuclear Magnetic Resonance. **2020**, 13, 108-118		10
284	Low-level LIBS and Raman data fusion in the context of in situ Mars exploration. **2020**, 51, 1682-1701		7

283	Using Short-wave Infrared Range Spectrometry Data to Determine Brick Characteristics. **2020**, 14, 38-50		2
282	Bladder tissue characterization using probe-based Raman spectroscopy: Evaluation of tissue heterogeneity and influence on the model prediction. **2020**, 13, e201960025		16
281	Pre-meal protein intake alters postprandial plasma metabolome in subjects with metabolic syndrome. **2020**, 59, 1881-1894		4
280	Identification of Genuine and Adulterated Pinellia ternata by Mid-Infrared (MIR) and Near-Infrared (NIR) Spectroscopy with Partial Least Squares - Discriminant Analysis (PLS-DA). *Analytical Letters*, **2020**, 53, 937-959	2.2	8
279	Evaluation and improvement of model robustness for plastics samples classification by laser-induced breakdown spectroscopy. **2020**, 125, 106035		9
278	Rhodnius spp. are differentiated based on the peptide/protein profile by matrix-assisted laser desorption/ionization mass spectrometry and chemometric tools. **2020**, 412, 1431-1439		7
277	Spectrochemical differentiation of meningioma tumours based on attenuated total reflection Fourier-transform infrared (ATR-FTIR) spectroscopy. **2020**, 412, 1077-1086		8
276	Detection and quantification of adulterants in honey by LIBS. **2020**, 311, 125886		22
275	Effects of land-use conversions on the ecosystem services in the agro-pastoral ecotone of northern China. **2020**, 249, 119360		30
274	Chemometrics in Forensics. **2020**, 113-148		1
273	Sparse Projection Pursuit Analysis: An Alternative for Exploring Multivariate Chemical Data. *Analytical Chemistry*, **2020**, 92, 1755-1762	7.8	5
272	Metabolic fingerprints discriminating severity of acute ischemia using in vivo high-field H magnetic resonance spectroscopy. **2020**, 152, 252-262		
271	Classification of tropical hardwood samples by species and geographical origin. *Microchemical Journal*, **2020**, 159, 105326	4.8	1
270	Classification of printing inks in pharmaceutcal packages by Laser-Induced Breakdown Spectroscopy and Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy. **2020**, 172, 105963		3
269	Proximal colon-derived O-glycosylated mucus encapsulates and modulates the microbiota. **2020**, 370, 467-472		47
268	Partial Least-Squares Discriminant Analysis and Ensemble-Based Flexible Docking of PD-1/PD-L1 Inhibitors: A Pilot Study. **2020**, 5, 26914-26923		2
267	Rapid Analytical Method to Characterize the Freshness of Olive Oils Using Fluorescence Spectroscopy and Chemometric Algorithms. **2020**, 2020, 8860161		10
266	Criteria for comparing infrared spectra A review of the forensic and analytical chemistry literature. *Forensic Chemistry*, **2020**, 18, 100224	2.8	5

265	A pilot study for early detection of oral premalignant diseases using oral cytology and Raman micro-spectroscopy: Assessment of confounding factors. **2020**, 13, e202000079		6
264	A three-dimensional discriminant analysis approach for hyperspectral images. **2020**, 145, 5915-5924		2
263	Complex Chemical Data Classification and Discrimination Using Locality Preserving Partial Least Squares Discriminant Analysis. **2020**, 5, 26601-26610		6
262	Application of luminescent markers to ammunition encoding in forensic routine using a Video Spectral Comparator (VSC). *Microchemical Journal*, **2020**, 159, 105362	4.8	1
261	Vibrational spectroscopy of liquid biopsies for prostate cancer diagnosis. **2020**, 12, 1758835920918499		13
260	Defining Surface Types of Mars Using Global CRISM Summary Product Maps. **2020**, 125, e2019JE006337		4
259	Whole-blood expression of inflammasome- and glucocorticoid-related mRNAs correctly separates treatment-resistant depressed patients from drug-free and responsive patients in the BIODEP study. **2020**, 10, 232		36
258	Analysis of Lipidome Disclosed Differences Among the Species and Reveals Presence of Unusual Yeast Lipids. **2020**, 10, 338		5
257	Hyperspectral imaging for identification of Zebra Chip disease in potatoes. **2020**, 197, 306-317		11
256	1H NMR-based metabonomics for infertility diagnosis in men with varicocele. **2020**, 37, 2233-2247		6
255	Classification of Mosquitoes with Infrared Spectroscopy and Partial Least Squares-Discriminant Analysis. **2020**, 74, 900-912		2
254	Gas sensors based on mass-sensitive transducers. Part 2: Improving the sensors towards practical application. **2020**, 412, 6707-6776		3
253	Vibrational Spectroscopy Coupled to a Multivariate Analysis Tiered Approach for Argentinean Honey Provenance Confirmation. **2020**, 9,		3
252	Using chemometrics to characterise and unravel the near infra-red spectral changes induced in aubergine fruit by chilling injury as influenced by storage time and temperature. **2020**, 198, 137-146		6
251	Analysis of Raman spectra for the verification of Australian grass- and grain-fed beef using principal component analysis and partial least square models. **2020**, 51, 2338-2346		4
250	Classification and Quantification of Microplastics (. *Analytical Chemistry*, **2020**, 92, 13724-13733	7.8	37
249	Non-Destructive Identification and Estimation of Granulation in Honey Pomelo Using Visible and Near-Infrared Transmittance Spectroscopy Combined with Machine Vision Technology. **2020**, 10, 5399		4
248	C NMR-Based Chemical Fingerprint for the Varietal and Geographical Discrimination of Wines. **2020**, 9,		8

247	Molecular fluorescence spectroscopy with multi-way analysis techniques detects spectral variations distinguishing uninfected serum versus dengue or chikungunya viral infected samples. **2020**, 10, 13758		5
246	Expansion of Human Limbal Epithelial Stem/Progenitor Cells Using Different Human Sera: A Multivariate Statistical Analysis. **2020**, 21,		0
245	Early detection of black Sigatoka in banana leaves using hyperspectral images. **2020**, 8, e11383		5
244	New Variants of Global-Local Partial Least Squares Discriminant Analysis for Appearance-Based Face Recognition. **2020**, 8, 166703-166720		1
243	Wavelength Selection FOR Rapid Identification of Different Particle Size Fractions of Milk Powder Using Hyperspectral Imaging. *Sensors*, **2020**, 20,	3.8	8
242	Potential of the Electronic Nose for the Detection of Respiratory Diseases with and without Infection. **2020**, 21,		8
241	So you think you can PLS-DA?. **2020**, 21, 2		44
240	Multianalyzer Spectroscopic Data Fusion for Soil Characterization. **2020**, 10, 8723		0
239	Predicting ionic liquid melting points using machine learning. **2020**, 114686		0
238	Plasma spectroscopy + chemometrics: An ideal approach for the spectrochemical analysis of iron phosphate glass samples. *Journal of Chemometrics*, **2020**, 34, e3310	1.6	2
237	A perfect tandem: chemometric methods and microfluidic colorimetric twin sensors on paper. Beyond the traditional analytical approach. *Microchemical Journal*, **2020**, 157, 104930	4.8	1
236	Sensing Polymer/Paracetamol Interaction with an Independent Component Analysis-Based SERS-MIP Nanosensor. **2020**, 15, 1533-1539		7
235	Metabolomics and Multi-Omics Integration: A Survey of Computational Methods and Resources. **2020**, 10,		33
234	Aberrant inflammatory profile in acute but not recovered anorexia nervosa. **2020**, 88, 718-724		13
233	Compliance with EU vs. extra-EU labelled geographical provenance in virgin olive oils: A rapid untargeted chromatographic approach based on volatile compounds. **2020**, 130, 109566		7
232	Combined Machine Learning and Molecular Modelling Workflow for the Recognition of Potentially Novel Fungicides. *Molecules*, **2020**, 25,	4.8	0
231	Multivariate optimization of an analytical method for the analysis of Abruzzo white wines by ICP OES. **2020**, 12, 2772-2778		5
230	Medical Applications of Raman Spectroscopy. **2020**, 1-21		1

229	Correlation and association analyses in microbiome study integrating multiomics in health and disease. **2020**, 171, 309-491		24
228	Stable isotope ratio analysis combined with inductively coupled plasma-mass spectrometry for geographical discrimination between Italian and foreign saffron. **2020**, 55, e4595		6
227	ATR-MIR spectroscopy to predict commercial milk major components: A comparison between a handheld and a benchtop instrument. **2020**, 200, 103995		10
226	Tutorial: multivariate classification for vibrational spectroscopy in biological samples. **2020**, 15, 2143-2162		73
225	Integrated biomarker for type 2 diabetes mellitus and impaired fasting glucose based on metabolomics analysis using ultra-high performance liquid chromatography quadrupole-Orbitrap high-resolution accurate mass spectrometry. **2020**, 34, e8779		5
224	A chemometric-assisted voltammetric analysis of free and Zn(II)-loaded metallothionein-3 states. **2020**, 134, 107501		4
223	RGCxGC toolbox: An R-package for data processing in comprehensive two-dimensional gas chromatography-mass spectrometry. *Microchemical Journal*, **2020**, 156, 104830	4.8	13
222	Respirator usage protects brain white matter from welding fume exposure: A pilot magnetic resonance imaging study of welders. **2020**, 78, 202-208		0
221	Extended preclinical investigation of lactate for neuroprotection after ischemic stroke. **2020**, 4, 2514183X2090457		4
220	Discrimination of Potato (Solanum tuberosum L.) Accessions Collected in Majella National Park (Abruzzo, Italy) Using Mid-Infrared Spectroscopy and Chemometrics Combined with Morphological and Molecular Analysis. **2020**, 10, 1630		7
219	Vibrational spectroscopy in protein research toward virus identification: challenges, new research, and future perspectives. **2020**, 315-335		0
218	Raman microspectroscopic study for the detection of oral field cancerisation using brush biopsy samples. **2020**, 13, e202000131		4
217	Feasibility of precise and reliable glucose quantification in human whole blood samples by 1 tesla benchtop NMR. **2020**, 33, e4358		2
216	Flash Gas Chromatography in Tandem with Chemometrics: A Rapid Screening Tool for Quality Grades of Virgin Olive Oils. **2020**, 9,		11
215	Liquid chromatographic methods coupled to chemometrics: a short review to present the key workflow for the investigation of wine phenolic composition as it is affected by environmental factors. *Environmental Science and Pollution Research*, **2021**, 28, 59150-59164	5.1	11
214	Geographical discrimination and authentication of lentils (Lens culinaris Medik.) by ICP-OES elemental analysis and chemometrics. **2020**, 118, 107438		6
213	Recent applications of chemometrics in one- and two-dimensional chromatography. **2020**, 43, 1678-1727		17
212	Using the Best-fit approach to investigate the effects of politico-economic and social barriers on SMEs' internationalization in an emerging country context: Implications and future directions. **2020**, 62, 199-211		12

211	Variable importance: Comparison of selectivity ratio and significance multivariate correlation for interpretation of latent-variable regression models. *Journal of Chemometrics*, **2020**, 34, e3211	1.6	7
210	Composition of cometary particles collected during two periods of the Rosetta mission: multivariate evaluation of mass spectral data. *Journal of Chemometrics*, **2020**, 34, e3218	1.6	
209	Modelling the vigour of maize seeds submitted to artificial accelerated ageing based on ATR-FTIR data and chemometric tools (PCA, HCA and PLS-DA). **2020**, 6, e03477		12
208	Chamber-to-Chamber Discrepancy Detection in Semiconductor Manufacturing. **2020**, 33, 86-95		4
207	Novel Kernel Orthogonal Partial Least Squares for Dominant Sensor Data Extraction. **2020**, 8, 36131-36139		2
206	Rapid and Nondestructive Discrimination of Geographical Origins of Longjing Tea using Hyperspectral Imaging at Two Spectral Ranges Coupled with Machine Learning Methods. **2020**, 10, 1173		11
205	Methods for Early Detection of Microbiological Infestation of Buildings Based on Gas Sensor Technologies. **2020**, 8, 7		8
204	Analysis of Vegetable Oil from Different Suppliers by Chemometric Techniques to Ensure Correct Classification of Oil Sources to Deal with Counterfeiting. **2020**, 13, 1138-1147		5
203	Multiplex Surface-Enhanced Raman Scattering Identification and Quantification of Urine Metabolites in Patient Samples within 30 min. *ACS Nano*, **2020**, 14, 2542-2552	16.7	44
202	Reduced scale model qualification of 5-L and 250-ml bioreactors using multivariant visualization and Bayesian inferential methods. **2020**, 117, 1337-1347		
201	New insights into the evolutionary features of viral overlapping genes by discriminant analysis. **2020**, 546, 51-66		19
200	Metabolic Fingerprinting with Fourier-Transform Infrared (FTIR) Spectroscopy: Towards a High-Throughput Screening Assay for Antibiotic Discovery and Mechanism-of-Action Elucidation. **2020**, 10,		9
199	Implementation of Multispectral Imaging (MSI) for Microbiological Quality Assessment of Poultry Products. **2020**, 8,		6
198	Trace element signatures in hematite and goethite associated with the KiggavikÅndrew Lake structural trend U deposits (Nunavut, Canada). *Mineralium Deposita*, **2021**, 56, 509-535	4.8	4
197	Fractional order modeling and recognition of nitrogen content level of rubber tree foliage. **2021**, 29, 42-52		5
196	Rapid discrimination of intact beef, venison and lamb meat using Raman spectroscopy. **2021**, 343, 128441		6
195	Predictive identification of co-formers in co-amorphous systems. **2021**, 157, 105636		4
194	Hyperspectral imaging coupled with multivariate methods for seed vitality estimation and forecast for Quercus variabilis. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 245, 118888	4.4	9

193   Mass spectrometry-based untargeted metabolomics approach for differentiation of beef of different geographic origins. **2021**, 338, 127847   15

192   Application of near-infrared hyperspectral (NIR) images combined with multivariate image analysis in the differentiation of two mycotoxicogenic Fusarium species associated with maize. **2021**, 344, 128615   9

191   In vivo toxicometabolomics reveals multi-organ and urine metabolic changes in mice upon acute⬜exposure to human-relevant doses of 3,4-methylenedioxypyrovalerone (MDPV). **2021**, 95, 509-527   3

190   Qualitative pattern recognition in chemistry: Theoretical background and practical guidelines. *Microchemical Journal*, **2021**, 162, 105725   4.8   14

189   A comparative analysis of different biofluids towards ovarian cancer diagnosis using Raman microspectroscopy. **2021**, 413, 911-922   6

188   Spectralprint techniques for wine and vinegar characterization, authentication and quality control: Advances and projections. **2021**, 134, 116121   17

187   Infrared Spectroscopy of Blood. **2021**, 75, 611-646   12

186   A comparative analysis of different biofluids using Raman spectroscopy to determine disease activity in ANCA-associated vasculitis. **2021**, 14, e202000426   1

185   Novel chiral voltammetric sensor for tryptophan enantiomers based on 3-neomenthylindene as recognition element. **2021**, 880, 114939   10

184   Multivariate classification for the direct determination of cup profile in coffee blends via handheld near-infrared spectroscopy. **2021**, 222, 121526   9

183   Prediction of pathological response to neo-adjuvant chemoradiotherapy for oesophageal cancer using vibrational spectroscopy. **2021**, 3, e202000014   0

182   Estimating Soil Properties and Classes from Spectra. **2021**, 165-214

181   Canopy spectral reflectance detects oak wilt at the landscape scale using phylogenetic discrimination.   2

180   Detection of Plant-Derived Adulterants in Saffron (Crocus sativus L.) by HS-SPME/GC-MS Profiling of Volatiles and Chemometrics. **2021**, 14, 784-796   3

179   Assessment of the Kernel Gram Matrix Representation of Data in Order to Avoid the Alignment of Chromatographic Signals. *Molecules*, **2021**, 26,   4.8

178   Chromatographic methods. **2021**, 65-99

177   Nontargeted fingerprinting approaches. **2021**, 163-193   1

176   Performance Evaluation of Classical Classifiers and Deep Learning Approaches for Polymers Classification Based on Hyperspectral Images. **2021**, 281-292   3

175	Cerebral arterial architectonics and CFD simulation in mice with type 1 diabetes mellitus of different duration. **2021**, 11, 3969	3
174	Chemometric applications in metabolomic studies using chromatography-mass spectrometry. **2021**, 135, 116165	9
173	Suitability of sugar, amino acid, and inorganic ion compositions to distinguish fir and spruce honey. **2021**, 247, 879-888	1
172	A guide to good practice in chemometric methods for vibrational spectroscopy, electrochemistry, and hyphenated mass spectrometry. **2021**, 135, 116157	14
171	Classification of Southern Australian Grass- and Grain-Fed Beef. **2021**, 14, 1730-1743	1
170	Lithology Discrimination Using Sentinel-1 Dual-Pol Data and SRTM Data. **2021**, 13, 1280	5
169	Evaluation of adulteration in distillate samples of Rosa damascena Mill using colorimetric sensor arrays, chemometric tools and dispersive liquid-liquid microextraction-GC-MS. **2021**, 32, 1027-1038	1
168	Defining Eucalyptus urophylla with its hybrid and the rules of genetic recombination using near infrared spectroscopy. **2021**, 29, 236-244	0
167	Multivariate statistical analysis of trace element compositions of native gold from orogenic gold deposits: Implication for mineral exploration. **2021**, 131, 104061	8
166	The Use of Multispectral Imaging and Single Seed and Bulk Near-Infrared Spectroscopy to Characterize Seed Covering Structures: Methods and Applications in Seed Testing and Research. **2021**, 11, 301	8
165	Untargeted metabolomics for uncovering plasma biological markers of wet age-related macular degeneration. **2021**, 13, 13968-14000	4
164	In Vitro 1H NMR Metabolic Profiles of Liver, Brain, and Serum in Rats After Chronic Consumption of Alcohol. **2021**, 52, 661-675	0
163	Origin, Evolution and Stability of Overlapping Genes in Viruses: A Systematic Review. **2021**, 12,	5
162	Distinguishing active from quiescent disease in ANCA-associated vasculitis using attenuated total reflection Fourier-transform infrared spectroscopy. **2021**, 11, 9981	1
161	Supervised dimensionality reduction for big data. **2021**, 12, 2872	3
160	Geochemical signatures in native gold derived from Au-bearing ore deposits. **2021**, 132, 104066	6
159	Lake snow caused by the invasive diatom Lindavia intermedia can be discriminated from different sites and from other algae using vibrational spectroscopy.	2
158	Raman spectral cytopathology for cancer diagnostic applications. **2021**, 16, 3716-3735	6

157	Backstepping Methodology to Troubleshoot Plant-Wide Batch Processes in Data-Rich Industrial Environments. **2021**, 9, 1074		1
156	Intraspecific variation in polar and nonpolar metabolite profiles of a threatened Caribbean coral. **2021**, 17, 60		2
155	Towards development of a novel screening method for identifying Alzheimer's disease risk: Raman spectroscopy of blood serum and machine learning. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 254, 119603	4.4	4
154	Raman spectroscopy of blood and urine liquid biopsies for ovarian cancer diagnosis: identification of chemotherapy effects. **2021**, 14, e202100195		0
153	Authentication of Douro DO monovarietal red wines based on anthocyanin profile: Comparison of partial least squares discriminant analysis, decision trees and artificial neural networks. **2021**, 125, 107979		2
152	Line-scan Raman scattering image and multivariate analysis for rapid and noninvasive detection of restructured beef. **2021**, 60, 6357-6365		1
151	Effects of Urbanization on Ecosystem Services in the Shandong Peninsula Urban Agglomeration, in China: The Case of Weifang City. **2021**, 5, 54		3
150	Detection of ovarian cancer (neo-adjuvant chemotherapy effects) via ATR-FTIR spectroscopy: comparative analysis of blood and urine biofluids in a large patient cohort. **2021**, 413, 5095-5107		5
149	PPAR-induced changes in visceral fat and adiponectin levels are associated with improvement of steatohepatitis in patients with NASH. **2021**, 41, 2659-2670		13
148	Non-target protein analysis of samples from wastewater treatment plants using the regions of interest-multivariate curve resolution (ROIMCR) chemometrics method. **2021**, 9, 105752		8
147	Individualized diversity in the extracellular metabolome of live human gliomas.		
146	Validation and analysis of the geographical origin of (Oliv.) Diels using multi-element and stable isotopes. **2021**, 9, e11928		1
145	HPLC Fingerprints for the Characterization of Walnuts and the Detection of Fraudulent Incidents. **2021**, 10,		2
144	PLS for classification. **2021**, 216, 104374		5
143	Isolating the white matter circuitry of the dorsal language stream: Connectome-Symptom Mapping in stroke induced aphasia. **2021**, 42, 5689-5702		3
142	Chemical imaging and machine learning for sub-classification of oesophageal tissue histology. e202100004		0
141	Recycling-Oriented Characterization of Post-Earthquake Building Waste by Different Sensing Techniques. **2021**, 7,		2
140	Metabolomics approach to study in vivo toxicity of graphene oxide nanosheets. **2021**,		1

139	GC-MS urinary metabolomics analysis of inherited metabolic diseases and stable metabolic biomarker screening by a comprehensive chemometric method. *Microchemical Journal*, **2021**, 168, 106350	4.8	0
138	Classification of cytological samples from oral potentially malignant lesions through Raman spectroscopy: A pilot study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2022**, 266, 120437	4.4	0
137	Biofluid analysis and classification using IR and 2D-IR spectroscopy. **2021**, 217, 104408		1
136	Chemometric strategies for authenticating extra virgin olive oils from two geographically adjacent Catalan protected designations of origin. *Microchemical Journal*, **2021**, 169, 106611	4.8	1
135	Improved multi-class discrimination by Common-Subset-of-Independent-Variables Partial-Least-Squares Discriminant Analysis. **2021**, 234, 122595		2
134	A novel analytical strategy for discriminating antibiotic mycelial residue adulteration in feed based on ATR-IR and microscopic infrared imaging. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 261, 120060	4.4	1
133	Exploring the volatile metabolome of conventional and organic walnut oils by solid-phase microextraction and analysis by GC-MS combined with chemometrics. **2021**, 363, 130331		7
132	Classification of rice based on storage time by using near infrared spectroscopy and chemometric methods. *Microchemical Journal*, **2021**, 171, 106841	4.8	3
131	Correction of the moisture variation in wood NIR spectra for species identification using EPO and soft PLS2-DA. *Microchemical Journal*, **2021**, 171, 106839	4.8	0
130	Machine learning-based chemometric methods for quality and authentication of milk and dairy products. **2022**, 261-280		
129	Detection of adulterations in a valuable Brazilian honey by using spectrofluorimetry and multiway classification. **2022**, 370, 131064		2
128	Features Selection and Extraction in Statistical Analysis of Proteomics Datasets. **2021**, 2361, 143-159		0
127	Simultaneous elucidation of antibiotic mechanism of action and potency with high-throughput Fourier-transform infrared (FTIR) spectroscopy and machine learning. **2021**, 105, 1269-1286		4
126	Glycerophospholipid and detoxification pathways associated with small for gestation age pathophysiology: discovery metabolomics analysis in the SCOPE cohort. **2021**, 17, 5		2
125	Identification of a Zika NS2B epitope as a biomarker for severe clinical phenotypes. **2021**, 12, 1525-1539		1
124	Skeletal Muscle Metabolomics for Metabolic Phenotyping and Biomarker Discovery. **2019**, 193-217		1
123	Sampling, Detection, Identification, and Analysis of Bacterial Volatile Organic Compounds (VOCs). **2020**, 281-304		1
122	Application of Chemometrics in the Food Sciences. **2020**, 99-111		2

121	Stable isotope resolved metabolomics classification of prostate cancer cells using hyperpolarized NMR data. **2020**, 316, 106750	2
120	Disentangling metabolic functions of bacteria in the honey bee gut.	4
119	So you think you can PLS-DA?.	3
118	Brain dynamics and temporal trajectories during task and naturalistic processing.	1
117	Peripheral blood cell immunophenotyping reveals distinct subgroups of inflamed depression.	0
116	Disentangling metabolic functions of bacteria in the honey bee gut. **2017**, 15, e2003467	149
115	Prediction of preeclampsia risk in first time pregnant women: Metabolite biomarkers for a clinical test. **2020**, 15, e0244369	3
114	Detection of Wastewater Treatment Process Disturbances in Bioreactors Using the E-Nose Technology. **2018**, 25, 405-418	3
113	The assessment of metabolite alteration induced by -OH functionalized multi-walled carbon nanotubes in mice using NMR-based metabonomics. **2018**, 8, 107-116	4
112	Wood species identification from Atlantic forest by near infrared spectroscopy. **2019**, 28, e015	5
111	Development of computational models using omics data for the identification of effective cancer metabolic biomarkers. **2021**, 17, 881-893	0
110	Soybean Processing Wastes: Novel Insights on Their Production, Extraction of Isoflavones, and Their Therapeutic Properties. **2021**,	3
109	The Hitchhiker's Guide to Untargeted Lipidomics Analysis: Practical Guidelines. **2021**, 11,	1
108	Evaluation of classifier performance for multiclass phenotype discrimination in untargeted metabolomics.	
107	Towards Raman-Based Screening of Acute Lymphoblastic Leukemia-Type B (B-ALL) Subtypes. **2021**, 13,	1
106	Discriminating tropical grasses grown under different nitrogen fertilizer regimes in KwaZulu-Natal, South Africa. **2020**, 147-163	
105	Identification of cellulose textile fibers. **2021**, 146, 7503-7509	1
104	Deep Learning Theoretical Chapter for Chemometrician. **2020**, 723-739	

103	Application of IR and UV–VIS spectroscopies and multivariate analysis for the classification of waste vegetable oils. **2022**, 178, 106088		1
102	Chemometrics in Bioanalytical Chemistry. **2022**, 497-541		0
101	Intrasexual cuticular hydrocarbon dimorphism in a wasp sheds light on hydrocarbon biosynthesis genes in Hymenoptera.		0
100	Deep-learning model observer for a low-contrast hepatic metastases localization task in computed tomography. **2021**,		2
99	FeatureEnVi: Visual Analytics for Feature Engineering Using Stepwise Selection and Semi-Automatic Extraction Approaches.. **2022**, PP,		3
98	Breath analysis using electronic nose and gas chromatography- mass spectrometry: a pilot study on bronchial infections in bronchiectasis.. *Clinica Chimica Acta*, **2021**,	6.2	1
97	Raman spectroscopy of fingerprints and chemometric analysis for forensic sex determination in humans. *Forensic Chemistry*, **2022**, 27, 100395	2.8	2
96	Serological diagnosis of strongyloidiasis in immunocompetent and immunosuppressed patients based on an electrochemical immunoassay using a flexible device allied to PLS-DA and ROC statistical tools. *Sensors and Actuators B: Chemical*, **2022**, 354, 131213	8.5	0
95	Study on the Establishment of Quality Discrimination Model of Longjing Green Tea. *SSRN Electronic Journal*,		1
94	Multiomics Analysis of Structural Magnetic Resonance Imaging of the Brain and Cerebrospinal Fluid Metabolomics in Cognitively Normal and Impaired Adults.. *Frontiers in Aging Neuroscience*, **2021**, 13, 796067	5.2	0
93	Application of multivariate data analysis for food quality investigations: An example-based review.. *Food Research International*, **2022**, 151, 110878	7	4
92	Obsidian source classification and defining local in early Holocene Southeast Alaska. *Geoarchaeology - an International Journal*,	1.4	0
91	Statistical methods for in silico tools used for risk assessment and toxicology. *ChemistrySelect*, **2022**,	1.8	
90	Noninvasive Diagnostic for COVID-19 from Saliva Biofluid via FTIR Spectroscopy and Multivariate Analysis.. *Analytical Chemistry*, **2022**,	7.8	2
89	Noninvasive and Point-of-Care Surface-Enhanced Raman Scattering (SERS)-Based Breathalyzer for Mass Screening of Coronavirus Disease 2019 (COVID-19) under 5 min.. *ACS Nano*, **2022**,	16.7	11
88	Assessing chemometric models developed using Raman spectroscopy and fatty acid data for Northern and Southern Australian beef production systems.. *Meat Science*, **2022**, 187, 108753	6.4	0
87	In situ imaging of lignin and related compounds by Raman, Fourier-transform infrared (FTIR) and fluorescence microscopy. *Advances in Botanical Research*, **2022**,	2.2	
86	Elemental Chemometrics as Tools to Depict Stalked Barnacle () Harvest Locations and Food Safety.. *Molecules*, **2022**, 27,	4.8	3

85	Multispectral Wavebands Selection for the Detection of Potential Foreign Materials in Fresh-Cut Vegetables.. *Sensors*, **2022**, 22,	3.8	0
84	Ensemble classification and regression techniques combined with portable near infrared spectroscopy for facile and rapid detection of water adulteration in bovine raw milk. *Journal of Chemometrics*,	1.6	0
83	Blood-based transcriptomic signature panel identification for cancer diagnosis: Benchmarking of feature extraction methods.		
82	Urinary metabolomic profiling from spontaneous tolerant kidney transplanted recipients shows enrichment in tryptophan-derived metabolites.. *EBioMedicine*, **2022**, 103844	8.8	1
81	Rapid Prediction of Fig Phenolic Acids and Flavonoids Using Mid-Infrared Spectroscopy Combined With Partial Least Square Regression.. *Frontiers in Plant Science*, **2022**, 13, 782159	6.2	1
80	Real-time adjustment of injection molding process settings by utilizing Design of Experiment, time series profiles and PLS-DA. *Quality Engineering*, 1-15	1.4	
79	Multielemental Inductively Coupled Plasma Optical Emission Spectrometric (ICP-OES) Method for the Determination of Nutrient and Toxic Elements in Wild Mushrooms Coupled to Unsupervised and Supervised Chemometric Tools for Their Classification by Species. *Analytical Letters*, 1-16	2.2	2
78	Methane detection to 1 ppm using machine learning analysis of atmospheric pressure plasma optical emission spectra. *Journal Physics D: Applied Physics*, **2022**, 55, 225205	3	
77	Behavioural Classification of Cattle Using Neck-Mounted Accelerometer-Equipped Collars.. *Sensors*, **2022**, 22,	3.8	1
76	Functional changes in neural mechanisms underlying post-traumatic stress disorder in World Trade Center responders.		
75	Variation of trace elements in chalcopyrite from worldwide Ni-Cu sulfide and Reef-type PGE deposits: implications for mineral exploration. *Mineralium Deposita*, 1	4.8	0
74	Multivariate tools to investigate the spatial contaminant distribution in a highly anthropized area (Gulf of Naples, Italy).. *Environmental Science and Pollution Research*, **2022**, 1	5.1	1
73	Comparative study on the real-time monitoring of a fluid bed drying process of extruded granules using near-infrared spectroscopy and audible acoustic emission.. *International Journal of Pharmaceutics*, **2022**, 121689	6.5	0
72	Near-infrared spectroscopy combined with chemometrics to classify cosmetic foundations from a crime scene. *Science and Justice - Journal of the Forensic Science Society*, **2022**, 62, 327-335	2	2
71	Canopy spectral reflectance detects oak wilt at the landscape scale using phylogenetic discrimination. *Remote Sensing of Environment*, **2022**, 273, 112961	13.2	0
70	Scott test associated with multivariate image analysis: A more selective alternative for cocaine research in forensic laboratories.. *Forensic Science International*, **2022**, 335, 111277	2.6	1
69	Ethyl carbamate regulate esters degradation by activating hydrolysis during Baijiu ripening. *Food Research International*, **2022**, 156, 111157	7	3
68	Revising Fourier-transform infrared (FT-IR) and Raman spectroscopy towards brain cancer detection.. *Photodiagnosis and Photodynamic Therapy*, **2022**, 102785	3.5	4

67	Fitting limit lines (envelope curves) to spreads of geoenvironmental data. *Progress in Physical Geography*, **2022**, 46, 272-290	3.5	
66	Clinical applications of spectroscopic techniques in conjunction with multivariate analysis in virus diagnosis. *Biomedical Spectroscopy and Imaging*, **2021**, 1-27	1.3	
65	An overview on multi-elemental profile integrated with chemometrics for food quality assessment: toward new challenges.. *Critical Reviews in Food Science and Nutrition*, **2022**, 1-21	11.5	2
64	Antioxidant and Antiglycation Effects of Water Infusion, Its Phenolic Components, and Respective Metabolites.. *Molecules*, **2022**, 27,	4.8	1
63	Data_Sheet_1.docx. **2020**,		
62	Table_1.xlsx. **2020**,		
61	Table_2.docx. **2020**,		
60	Table_3.docx. **2020**,		
59	Study on the establishment of quality discrimination model of Longjing 43 green tea (Camellia sinensis(L.) Kuntze). *Journal of Applied Research on Medicinal and Aromatic Plants*, **2022**, 100389	2.6	
58	Classifying waste wood from Amazonian species by near-infrared spectroscopy (NIRS) to improve charcoal production. *Renewable Energy*, **2022**,	8.1	0
57	Classification of tablet formulations by desorption electrospray ionisation mass spectrometry and transmission Raman spectroscopy. *Journal of Chemometrics*,	1.6	
56	CHAPTER 10. On-site Food Authenticity Testing: Advances in Miniaturization of Spectrometers and Machine Learning. *Food Chemistry, Function and Analysis*, **2022**, 211-241	0.6	
55	Comparison of Multivariate ANOVA-Based Approaches for the Determination of Relevant Variables in Experimentally Designed Metabolomic Studies. *Molecules*, **2022**, 27, 3304	4.8	0
54	Proteome changes in an aquatic invertebrate consumer in response to different nutritional stressors. *Oecologia*,	2.9	
53	Introducing SourceXplorer, an open-source statistical tool for guided lithic sourcing. *Journal of Archaeological Science*, **2022**, 144, 105626	2.9	1
52	Classification of local diesel fuels and simultaneous prediction of their physicochemical parameters using FTIR-ATR data and chemometrics. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2022**, 279, 121451	4.4	1
51	ATR-IR Spectroscopy Application to Diagnostic Screening of Advanced Endometriosis. *Oxidative Medicine and Cellular Longevity*, **2022**, 2022, 1-13	6.7	0
50	Machine Learning Assisted Handheld Confocal Raman Micro-Spectroscopy for Identification of Clinically Relevant Atopic Eczema Biomarkers. *Sensors*, **2022**, 22, 4674	3.8	1

49	Raman spectroscopy and multivariate analysis for identification and classification of pharmaceutical pain reliever tablets. *Journal of Chemometrics*,	1.6	0
48	Classification of Pummelo (Citrus grandis) Extracts through UV-VIS-Based Chemical Fingerprint. *Beverages*, **2022**, 8, 34	3.4	0
47	Combination of machine learning and intelligent sensors in real-time quality control of alcoholic beverages. *Food Science and Technology*, 42,	2	
46	Could QSOR Modelling and Machine Learning Techniques Be Useful to Predict Wine Aroma?. *Food and Bioprocess Technology*,	5.1	
45	Saliva may be a diagnostic source of quality of life in psoriasis measured by Fourier transform infrared spectroscopy (FTIR) and chemometrics. *Photodiagnosis and Photodynamic Therapy*, **2022**, 103017	2.5	1
44	Effect of 45 full-scale WWTPs on tropical receiving water bodies in Brazil by partial least squares-discriminant analysis. *Journal of Water Sanitation and Hygiene for Development*,	1.5	
43	Efficient mass spectrometric characterization and classification of methylmalonic aciduria subtypes through urinary and blood metabolic profiles fusion. *Microchemical Journal*, **2022**, 181, 107754	4.8	
42	NMR Metabolomics in Serum Fingerprinting of Schizophrenia Patients in a Serbian Cohort. **2022**, 12, 707		0
41	Plant spectra as integrative measures of plant phenotypes.		1
40	Convolutional neural networks to predict brain tumor grades and Alzheimer disease with MR spectroscopic imaging data. **2022**, 17, e0268881		1
39	Blood-based transcriptomic signature panel identification for cancer diagnosis: benchmarking of feature extraction methods.		0
38	A High-Fat Diet Disrupts Nerve Lipids and Mitochondrial Function in Murine Models of Neuropathy. 13,		0
37	Heritage and modern wheat varieties discrimination by volatiles profiling. Is it a matter of flavor?. **2023**, 401, 134142		0
36	Offline Breath Analysis: Standardization of Breath Sampling and Analysis Using Mass Spectrometry and Innovative Algorithms. **2022**,		0
35	Data analysis in SERS diagnostics. **2022**, 1-51		0
34	The Development of Honey Recognition Models Based on the Association between ATR-IR Spectroscopy and Advanced Statistical Tools. **2022**, 23, 9977		1
33	Where Nanosensors Meet Machine Learning: Prospects and Challenges in Detecting Disease X. **2022**, 16, 13279-13293		3
32	Quality classification of kiwifruit under different storage conditions based on deep learning and hyperspectral imaging technology.		0

31	Machine learning, artificial intelligence, and chemistry: how smart algorithms are reshaping simulation and the laboratory. **2022**,	0
30	Development of multivariate classification models for the diagnosis of dengue virus infection. **2022** , 103136	0
29	Spelt authenticity assessment using a rapid and simple Fourier transform infrared spectroscopy (FTIR) method combined to advanced chemometrics.	0
28	Machine Learning Assisted Real-Time Label-Free SERS Diagnoses of Malignant Pleural Effusion due to Lung Cancer. **2022**, 12, 940	1
27	Interpretable machine learning methods for predictions in systems biology from omics data. 9,	0
26	Partial Least Squares-Discriminant Analysis of the Major and Trace Elements and their Evolutionary Characteristics from the Jinchuan Ni-Cu-(PGE) Sulfide Deposit, NW China. **2022**, 12, 1301	0
25	Comparison of Portable and Benchtop Near-Infrared Spectrometers for the Detection of Citric Acid-adulterated Lime Juice: A Chemometrics Approach. **2022**, 21,	0
24	Recycling of used vegetable oils by powder adsorption. 0734242X2211353	0
23	Authentication of fish oil (omega-3) supplements using class-oriented chemometrics and comprehensive two-dimensional gas chromatography coupled to mass spectrometry.	1
22	Data fusion of electronic noses and electronic tongues aids in botanical origin identification on imbalanced Codonopsis Radix samples. **2022**, 12,	0
21	Multivariate statistical analysis of trace elements in apatite: Discrimination of apatite with different origins. **2023**, 153, 105269	1
20	Guidelines to build PLS-DA chemometric classification models using a GC-IMS method: Dry-cured ham as a case of study. **2023**, 7, 100175	0
19	Unveiling the Predisposing Factors for the Development of Branch Canker and Dieback in Avocado: A Case of Study in Chilean Orchards. **2022**, 8, 1121	0
18	Micro-Raman Analysis of Sperm Cells on Glass Slide: Potential Label-Free Assessment of Sperm DNA toward Clinical Applications. **2022**, 12, 1051	0
17	Insights into Biochemical Sources and Diffuse Reflectance Spectral Features for Colorectal Cancer Detection and Localization. **2022**, 14, 5715	0
16	A critical review of recent trends in sample classification using Laser-Induced Breakdown Spectroscopy (LIBS). **2022**, 116859	0
15	An Overview on the Application of Chemometrics Tools in Food Authenticity and Traceability. **2022**, 11, 3940	0
14	Metabolite profiling of leaves of three <i>Epilobium</i> species. **2022**, 20, 279-293	0

13	Classification of Systemic Lupus Erythematosus Using Raman Spectroscopy of Blood and Automated Computational Detection Methods: A Novel Tool for Future Diagnostic Testing. **2022**, 12, 3158	0
12	The nexus between research impact and sustainability assessment: From stakeholders perspective.	0
11	Hyperspectral Imaging Coupled with Multivariate Analyses for Efficient Prediction of Chemical, Biological and Physical Properties of Seafood Products.	0
10	Early Detection of Wireworm (Coleoptera: Elateridae) Infestation and Drought Stress in Maize Using Hyperspectral Imaging. **2023**, 13, 178	0
9	Advanced mass spectrometric and spectroscopic methods coupled with machine learning for in vitro diagnosis. 20220038	1
8	Cell Phase Identification in a Three-Dimensional Engineered Tumor Model by Infrared Spectroscopic Imaging.	0
7	Aroma modeling and quality evaluation of spearmint (Mentha spicata subsp. spicata) using electronic nose technology coupled with artificial intelligence algorithms. **2023**, 35, 100473	0
6	Intrasexual cuticular hydrocarbon dimorphism in a wasp sheds light on hydrocarbon biosynthesis genes in Hymenoptera. **2023**, 6,	0
5	Exploring the Use of Raman Spectroscopy and Covariate-Adjusted Multivariate Analysis for the Detection of Irradiated Blood. **2023**, 199,	0
4	Giardia duodenalis Colonization Slightly Affects Gut Microbiota and Hematological Parameters in Clinically Healthy Dogs. **2023**, 13, 958	0
3	Identifying the Dangshan Physiological Disease of Pear Woolliness Response via Feature-Level Fusion of Near-Infrared Spectroscopy and Visual RGB Image. **2023**, 12, 1178	0
2	Spectral classification by generative adversarial linear discriminant analysis. **2023**, 341129	0
1	Application of XGBoost for Fast Identification of Typical Industrial Organic Waste Samples with Near-Infrared Hyperspectral Imaging.	0