

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

98
papers

3,803
citations

34
h-index

59
g-index

103
ext. papers

4,641
ext. citations

5.6
avg, IF

5.6
L-index

#	Paper	IF	Citations
98	A tutorial review: Metabolomics and partial least squares-discriminant analysis--a marriage of convenience or a shotgun wedding. <i>Analytica Chimica Acta</i> , 2015 , 879, 10-23	6.6	478
97	Individual and gender fingerprints in human body odour. <i>Journal of the Royal Society Interface</i> , 2007 , 4, 331-40	4.1	252
96	On Splitting Training and Validation Set: A Comparative Study of Cross-Validation, Bootstrap and Systematic Sampling for Estimating the Generalization Performance of Supervised Learning. <i>Journal of Analysis and Testing</i> , 2018 , 2, 249-262	3.2	160
95	¹ H NMR, GC-ESI-TOFMS, and data set correlation for fruit metabolomics: application to spatial metabolite analysis in melon. <i>Analytical Chemistry</i> , 2009 , 81, 2884-94	7.8	131
94	Portable, quantitative detection of Bacillus bacterial spores using surface-enhanced Raman scattering. <i>Analytical Chemistry</i> , 2013 , 85, 3297-302	7.8	116
93	Support Vector Machines: A Recent Method for Classification in Chemometrics. <i>Critical Reviews in Analytical Chemistry</i> , 2006 , 36, 177-188	5.2	116
92	Influence of missing values substitutes on multivariate analysis of metabolomics data. <i>Metabolites</i> , 2014 , 4, 433-52	5.6	115
91	Quantitative Analysis of the Banned Food Dye Sudan-1 Using Surface Enhanced Raman Scattering with Multivariate Chemometrics. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 7285-7290	3.8	109
90	Ultrasensitive Colorimetric Detection of Murine Norovirus Using NanoZyme Aptasensor. <i>Analytical Chemistry</i> , 2019 , 91, 3270-3276	7.8	108
89	Non-invasive metabolomic analysis of breath using differential mobility spectrometry in patients with chronic obstructive pulmonary disease and healthy smokers. <i>Analyst, The</i> , 2010 , 135, 315-20	5	106
88	A comparison of Raman and FT-IR spectroscopy for the prediction of meat spoilage. <i>Food Control</i> , 2013 , 29, 461-470	6.2	90
87	Fourier transform infrared spectroscopy and multivariate analysis for the detection and quantification of different milk species. <i>Journal of Dairy Science</i> , 2010 , 93, 5651-60	4	88
86	A comparative investigation of modern feature selection and classification approaches for the analysis of mass spectrometry data. <i>Analytica Chimica Acta</i> , 2014 , 829, 1-8	6.6	81
85	Analysis of volatile organic compounds in human saliva by a static sorptive extraction method and gas chromatography-mass spectrometry. <i>Journal of Chemical Ecology</i> , 2010 , 36, 1035-42	2.7	69
84	Absolute Quantification of Uric Acid in Human Urine Using Surface Enhanced Raman Scattering with the Standard Addition Method. <i>Analytical Chemistry</i> , 2017 , 89, 2472-2477	7.8	67
83	MALDI-MS and multivariate analysis for the detection and quantification of different milk species. <i>Analytical and Bioanalytical Chemistry</i> , 2011 , 399, 3491-502	4.4	63
82	Fourier transform infrared and Raman spectroscopies for the rapid detection, enumeration, and growth interaction of the bacteria <i>Staphylococcus aureus</i> and <i>Lactococcus lactis</i> ssp. <i>cremoris</i> in milk. <i>Analytical Chemistry</i> , 2011 , 83, 5681-7	7.8	59

81	Novel noninvasive identification of biomarkers by analytical profiling of chronic wounds using volatile organic compounds. <i>Wound Repair and Regeneration</i> , 2010 , 18, 391-400	3.6	58
80	Pattern recognition of gas chromatography mass spectrometry of human volatiles in sweat to distinguish the sex of subjects and determine potential discriminatory marker peaks. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2007 , 87, 161-172	3.8	53
79	Detection and quantification of bacterial spoilage in milk and pork meat using MALDI-TOF-MS and multivariate analysis. <i>Analytical Chemistry</i> , 2012 , 84, 5951-8	7.8	52
78	Metabolomics in melon: a new opportunity for aroma analysis. <i>Phytochemistry</i> , 2014 , 99, 61-72	4	51
77	Acclimation of metabolism to light in <i>Arabidopsis thaliana</i> : the glucose 6-phosphate/phosphate translocator GPT2 directs metabolic acclimation. <i>Plant, Cell and Environment</i> , 2015 , 38, 1404-17	8.4	51
76	The influence of scaling metabolomics data on model classification accuracy. <i>Metabolomics</i> , 2015 , 11, 684-695	4.7	48
75	Quantitative Online Liquid Chromatography-Surface-Enhanced Raman Scattering (LC-SERS) of Methotrexate and its Major Metabolites. <i>Analytical Chemistry</i> , 2017 , 89, 6702-6709	7.8	44
74	Discovery of Volatile Biomarkers of Parkinson's Disease from Sebum. <i>ACS Central Science</i> , 2019 , 5, 599-606	6.8	44
73	Surveillance for lower airway pathogens in mechanically ventilated patients by metabolomic analysis of exhaled breath: a case-control study. <i>Thorax</i> , 2015 , 70, 320-5	7.3	43
72	Through-container, extremely low concentration detection of multiple chemical markers of counterfeit alcohol using a handheld SORS device. <i>Scientific Reports</i> , 2017 , 7, 12082	4.9	42
71	Comparison of human axillary odour profiles obtained by gas chromatography/mass spectrometry and skin microbial profiles obtained by denaturing gradient gel electrophoresis using multivariate pattern recognition. <i>Metabolomics</i> , 2007 , 3, 427-437	4.7	40
70	VOC-based metabolic profiling for food spoilage detection with the application to detecting <i>Salmonella typhimurium</i> -contaminated pork. <i>Analytical and Bioanalytical Chemistry</i> , 2010 , 397, 2439-49	4.4	39
69	Multiblock principal component analysis: an efficient tool for analyzing metabolomics data which contain two influential factors. <i>Metabolomics</i> , 2012 , 8, 37-51	4.7	37
68	Simultaneous multiplexed quantification of nicotine and its metabolites using surface enhanced Raman scattering. <i>Analyst, The</i> , 2014 , 139, 4820-7	5	36
67	Rapid, accurate, and comparative differentiation of clinically and industrially relevant microorganisms via multiple vibrational spectroscopic fingerprinting. <i>Analyst, The</i> , 2016 , 141, 5127-36	5	35
66	Metabolic dysregulation in vitamin E and carnitine shuttle energy mechanisms associate with human frailty. <i>Nature Communications</i> , 2019 , 10, 5027	17.4	35
65	Rapid, Accurate, and Quantitative Detection of Propranolol in Multiple Human Biofluids via Surface-Enhanced Raman Scattering. <i>Analytical Chemistry</i> , 2016 , 88, 10884-10892	7.8	35
64	Consensus multivariate methods in gas chromatography mass spectrometry and denaturing gradient gel electrophoresis: MHC-congenic and other strains of mice can be classified according to the profiles of volatiles and microflora in their scent-marks. <i>Analyst, The</i> , 2009 , 134, 114-23	5	34

63	Rapid through-container detection of fake spirits and methanol quantification with handheld Raman spectroscopy. <i>Analyst, The</i> , 2018 , 144, 324-330	5	31
62	Simultaneous multiplexed quantification of caffeine and its major metabolites theobromine and paraxanthine using surface-enhanced Raman scattering. <i>Analytical and Bioanalytical Chemistry</i> , 2015 , 407, 8253-61	4.4	30
61	Combining metabolic fingerprinting and footprinting to understand the phenotypic response of HPV16 E6 expressing cervical carcinoma cells exposed to the HIV anti-viral drug lopinavir. <i>Analyst, The</i> , 2010 , 135, 1235-44	5	30
60	The challenge of applying Raman spectroscopy to monitor recombinant antibody production. <i>Analyst, The</i> , 2013 , 138, 6977-85	5	28
59	Application of dissimilarity indices, principal coordinates analysis, and rank tests to peak tables in metabolomics of the gas chromatography/mass spectrometry of human sweat. <i>Analytical Chemistry</i> , 2007 , 79, 5633-41	7.8	28
58	Optimization of matrix assisted desorption/ionization time of flight mass spectrometry (MALDI-TOF-MS) for the characterization of <i>Bacillus</i> and <i>Brevibacillus</i> species. <i>Analytica Chimica Acta</i> , 2014 , 840, 49-57	6.6	25
57	The optimisation of facile substrates for surface enhanced Raman scattering through galvanic replacement of silver onto copper. <i>Analyst, The</i> , 2012 , 137, 2791-8	5	24
56	Label-Free Surface Enhanced Raman Scattering Approach for High-Throughput Screening of Biocatalysts. <i>Analytical Chemistry</i> , 2016 , 88, 5898-903	7.8	24
55	Detection and quantification of the opioid tramadol in urine using surface enhanced Raman scattering. <i>Analyst, The</i> , 2015 , 140, 5965-70	5	23
54	Rapid, high-throughput, and quantitative determination of orange juice adulteration by Fourier-transform infrared spectroscopy. <i>Analytical Methods</i> , 2016 , 8, 5581-5586	3.2	23
53	Assessment of adaptive focused acoustics versus manual vortex/freeze-thaw for intracellular metabolite extraction from <i>Streptomyces lividans</i> producing recombinant proteins using GC-MS and multi-block principal component analysis. <i>Analyst, The</i> , 2010 , 135, 934-42	5	23
52	Intermittent energy restriction induces changes in breast gene expression and systemic metabolism. <i>Breast Cancer Research</i> , 2016 , 18, 57	8.3	22
51	Metabolic Profiling of <i>Geobacter sulfurreducens</i> during Industrial Bioprocess Scale-Up. <i>Applied and Environmental Microbiology</i> , 2015 , 81, 3288-98	4.8	21
50	Integrating multiple analytical platforms and chemometrics for comprehensive metabolic profiling: application to meat spoilage detection. <i>Analytical and Bioanalytical Chemistry</i> , 2013 , 405, 5063-74	4.4	20
49	Application of HPLC-PDA-MS metabolite profiling to investigate the effect of growth temperature and day length on blackcurrant fruit. <i>Metabolomics</i> , 2019 , 15, 12	4.7	18
48	Profiling of spatial metabolite distributions in wheat leaves under normal and nitrate limiting conditions. <i>Phytochemistry</i> , 2015 , 115, 99-111	4	18
47	Implementation of Fourier transform infrared spectroscopy for the rapid typing of uropathogenic <i>Escherichia coli</i> . <i>European Journal of Clinical Microbiology and Infectious Diseases</i> , 2014 , 33, 983-8	5.3	18
46	Untargeted metabolomics of COVID-19 patient serum reveals potential prognostic markers of both severity and outcome.. <i>Metabolomics</i> , 2021 , 18, 6	4.7	18

45	Probing the action of a novel anti-leukaemic drug therapy at the single cell level using modern vibrational spectroscopy techniques. <i>Scientific Reports</i> , 2017 , 7, 2649	4.9	17
44	Evaluation of metabolomics profiles of grain from maize hybrids derived from near-isogenic GM positive and negative segregant inbreds demonstrates that observed differences cannot be attributed unequivocally to the GM trait. <i>Metabolomics</i> , 2016 , 12, 82	4.7	17
43	Rapid Detection and Quantification of Novel Psychoactive Substances (NPS) Using Raman Spectroscopy and Surface-Enhanced Raman Scattering. <i>Frontiers in Chemistry</i> , 2019 , 7, 412	5	16
42	Optimization of XCMS parameters for LC-MS metabolomics: an assessment of automated versus manual tuning and its effect on the final results. <i>Metabolomics</i> , 2020 , 16, 14	4.7	16
41	Towards improved quantitative analysis using surface-enhanced Raman scattering incorporating internal isotope labelling. <i>Analytical Methods</i> , 2017 , 9, 6636-6644	3.2	15
40	Metabolomics investigation of recombinant mTNF α production in <i>Streptomyces lividans</i> . <i>Microbial Cell Factories</i> , 2015 , 14, 157	6.4	15
39	Dupuytren's disease metabolite analyses reveals alterations following initial short-term fibroblast culturing. <i>Molecular BioSystems</i> , 2012 , 8, 2274-88		15
38	Multiple metabolomics of uropathogenic <i>E. coli</i> reveal different information content in terms of metabolic potential compared to virulence factors. <i>Analyst, The</i> , 2014 , 139, 4193-9	5	14
37	Exploring the mode of action of dithranol therapy for psoriasis: a metabolomic analysis using HaCaT cells. <i>Molecular BioSystems</i> , 2015 , 11, 2198-209		14
36	Classification of <i>Bacillus</i> and <i>Brevibacillus</i> species using rapid analysis of lipids by mass spectrometry. <i>Analytical and Bioanalytical Chemistry</i> , 2016 , 408, 7865-7878	4.4	14
35	Metabolic profiling of meat: assessment of pork hygiene and contamination with <i>Salmonella typhimurium</i> . <i>Analyst, The</i> , 2011 , 136, 508-14	5	13
34	Methodological considerations for large-scale breath analysis studies: lessons from the U-BIOPRED severe asthma project. <i>Journal of Breath Research</i> , 2018 , 13, 016001	3.1	13
33	Imaging Isotopically Labeled Bacteria at the Single-Cell Level Using High-Resolution Optical Infrared Photothermal Spectroscopy. <i>Analytical Chemistry</i> , 2021 , 93, 3082-3088	7.8	13
32	Objective assessment of SERS thin films: comparison of silver on copper via galvanic displacement with commercially available fabricated substrates. <i>Analytical Methods</i> , 2017 , 9, 4783-4789	3.2	12
31	Diagnostic pattern recognition on gene-expression profile data by using one-class classification. <i>Journal of Chemical Information and Modeling</i> , 2005 , 45, 1392-401	6.1	12
30	Rapid UHPLC-MS metabolite profiling and phenotypic assays reveal genotypic impacts of nitrogen supplementation in oats. <i>Metabolomics</i> , 2019 , 15, 42	4.7	11
29	Chemometrics models for overcoming high between subject variability: applications in clinical metabolic profiling studies. <i>Metabolomics</i> , 2014 , 10, 375-385	4.7	11
28	A comparative study of cluster validation indices applied to genotyping data. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2005 , 78, 30-40	3.8	11

27	Untargeted metabolomics of COVID-19 patient serum reveals potential prognostic markers of both severity and outcome		11
26	pH plays a role in the mode of action of trimethoprim on Escherichia coli. <i>PLoS ONE</i> , 2018 , 13, e0200272	3.7	9
25	Real-Time Monitoring of Enzyme-Catalysed Reactions using Deep UV Resonance Raman Spectroscopy. <i>Chemistry - A European Journal</i> , 2017 , 23, 6983-6987	4.8	8
24	Metabolomic analysis of riboswitch containing E. coli recombinant expression system. <i>Molecular BioSystems</i> , 2016 , 12, 350-61		8
23	Compositional equivalence of grain from multi-trait drought-tolerant maize hybrids to a conventional comparator: univariate and multivariate assessments. <i>Journal of Agricultural and Food Chemistry</i> , 2014 , 62, 9597-608	5.7	8
22	Metabolomics Analysis Reveals the Participation of Efflux Pumps and Ornithine in the Response of Pseudomonas putida DOT-T1E Cells to Challenge with Propranolol. <i>PLoS ONE</i> , 2016 , 11, e0156509	3.7	8
21	Metabolic analysis of the response of DOT-T1E strains to toluene using Fourier transform infrared spectroscopy and gas chromatography mass spectrometry. <i>Metabolomics</i> , 2016 , 12, 112	4.7	7
20	A fuzzy distance metric for measuring the dissimilarity of planar chromatographic profiles with application to denaturing gradient gel electrophoresis data from human skin microbes: demonstration of an individual and gender-based fingerprint. <i>Analyst, The</i> , 2007 , 132, 638-46	5	7
19	Global metabolite profiles of rice brown planthopper-resistant traits reveal potential secondary metabolites for both constitutive and inducible defenses. <i>Metabolomics</i> , 2019 , 15, 151	4.7	7
18	Rapid Spectroscopic Liquid Biopsy for the Universal Detection of Brain Tumours. <i>Cancers</i> , 2021 , 13,	6.6	7
17	A workflow for bacterial metabolic fingerprinting and lipid profiling: application to Ciprofloxacin challenged Escherichia coli. <i>Metabolomics</i> , 2015 , 11, 438-453	4.7	6
16	A microbiome and metabolomic signature of phases of cutaneous healing identified by profiling sequential acute wounds of human skin: An exploratory study. <i>PLoS ONE</i> , 2020 , 15, e0229545	3.7	6
15	Rapid discrimination of Enterococcus faecium strains using phenotypic analytical techniques. <i>Analytical Methods</i> , 2016 , 8, 7603-7613	3.2	6
14	A metabolomics investigation into the effects of HIV protease inhibitors on HPV16 E6 expressing cervical carcinoma cells. <i>Molecular BioSystems</i> , 2014 , 10, 398-411		6
13	Partial Least Squares with Structured Output for Modelling the Metabolomics Data Obtained from Complex Experimental Designs: A Study into the Y-Block Coding. <i>Metabolites</i> , 2016 , 6,	5.6	6
12	Comparing root exudate collection techniques: An improved hybrid method. <i>Soil Biology and Biochemistry</i> , 2021 , 161, 108391	7.5	6
11	Phenotypic Characterisation of Shewanella oneidensis MR-1 Exposed to X-Radiation. <i>PLoS ONE</i> , 2015 , 10, e0131249	3.7	5
10	From Multistep Enzyme Monitoring to Whole-Cell Biotransformations: Development of Real-Time Ultraviolet Resonance Raman Spectroscopy. <i>Analytical Chemistry</i> , 2017 , 89, 12527-12532	7.8	4

9	Portable through Bottle SORS for the Authentication of Extra Virgin Olive Oil. <i>Applied Sciences (Switzerland)</i> , 2021 , 11, 8347	2.6	4
8	Phospholipidomics of peripheral blood mononuclear cells (PBMCs): the tricky case of children with autism spectrum disorder (ASD) and their healthy siblings. <i>Analytical and Bioanalytical Chemistry</i> , 2020 , 412, 6859-6874	4.4	3
7	Assessing the impact of nitrogen supplementation in oats across multiple growth locations and years with targeted phenotyping and high-resolution metabolite profiling approaches. <i>Food Chemistry</i> , 2021 , 355, 129585	8.5	3
6	Automated single-nucleotide polymorphism analysis using fluorescence excitation-emission spectroscopy and one-class classifiers. <i>Analytical and Bioanalytical Chemistry</i> , 2007 , 388, 655-64	4.4	2
5	Comparison of liver and plasma metabolic profiles in piglets of different ages as animal models for paediatric population. <i>Analyst, The</i> , 2020 , 145, 6859-6867	5	2
4	Metabolism in action: stable isotope probing using vibrational spectroscopy and SIMS reveals kinetic and metabolic flux of key substrates. <i>Analyst, The</i> , 2021 , 146, 1734-1746	5	2
3	Evaluation of Sample Preparation Methods for Inter-Laboratory Metabolomics Investigation of TK24. <i>Metabolites</i> , 2020 , 10,	5.6	1
2	PWE-200 Metabolomic profiling in pancreatic cancer; in search of new biomarkers. <i>Gut</i> , 2015 , 64, A300.1-A300	19.2	1
1	PTU-093 Metabolomic profiling in inflammatory bowel disease. <i>Gut</i> , 2015 , 64, A102.1-A102	19.2	1