Yun Xu

List of Publications by Year
in descending order

		94433	88630
101 papers	5,387 citations	37 h-index	70 g-index
103 all docs	103 docs citations	103 times ranked	8037 citing authors

#	Article	IF	Citations
1	Untargeted metabolomics of COVID-19 patient serum reveals potential prognostic markers of both severity and outcome. Metabolomics, 2022, 18, 6.	3.0	60
2	Rapid detection and quantification of the adulteration of orange juice with grapefruit juice using handheld Raman spectroscopy and multivariate analysis. Analytical Methods, 2022, 14, 1663-1670.	2.7	11
3	Simultaneous Raman and infrared spectroscopy: a novel combination for studying bacterial infections at the single cell level. Chemical Science, 2022, 13, 8171-8179.	7.4	22
4	Metabolism in action: stable isotope probing using vibrational spectroscopy and SIMS reveals kinetic and metabolic flux of key substrates. Analyst, The, 2021, 146, 1734-1746.	3.5	9
5	Imaging Isotopically Labeled Bacteria at the Single-Cell Level Using High-Resolution Optical Infrared Photothermal Spectroscopy. Analytical Chemistry, 2021, 93, 3082-3088.	6.5	41
6	Rapid Spectroscopic Liquid Biopsy for the Universal Detection of Brain Tumours. Cancers, 2021, 13, 3851.	3.7	22
7	Assessing the impact of nitrogen supplementation in oats across multiple growth locations and years with targeted phenotyping and high-resolution metabolite profiling approaches. Food Chemistry, 2021, 355, 129585.	8.2	8
8	Portable through Bottle SORS for the Authentication of Extra Virgin Olive Oil. Applied Sciences (Switzerland), 2021, 11, 8347.	2.5	11
9	Comparing root exudate collection techniques: An improved hybrid method. Soil Biology and Biochemistry, 2021, 161, 108391.	8.8	49
10	Optimization of XCMS parameters for LC–MS metabolomics: an assessment of automated versus manual tuning and its effect on the final results. Metabolomics, 2020, 16, 14.	3.0	33
11	Evaluation of Sample Preparation Methods for Inter-Laboratory Metabolomics Investigation of Streptomyces lividans TK24. Metabolites, 2020, 10, 379.	2.9	3
12	Phospholipidomics of peripheral blood mononuclear cells (PBMCs): the tricky case of children with autism spectrum disorder (ASD) and their healthy siblings. Analytical and Bioanalytical Chemistry, 2020, 412, 6859-6874.	3.7	7
13	Comparison of liver and plasma metabolic profiles in piglets of different ages as animal models for paediatric population. Analyst, The, 2020, 145, 6859-6867.	3.5	2
14	A microbiome and metabolomic signature of phases of cutaneous healing identified by profiling sequential acute wounds of human skin: An exploratory study. PLoS ONE, 2020, 15, e0229545.	2.5	24
15	Metabolic dysregulation in vitaminÂE and carnitine shuttle energy mechanisms associate with human frailty. Nature Communications, 2019, 10, 5027.	12.8	70
16	Rapid through-container detection of fake spirits and methanol quantification with handheld Raman spectroscopy. Analyst, The, 2019, 144, 324-330.	3.5	46
17	Rapid Detection and Quantification of Novel Psychoactive Substances (NPS) Using Raman Spectroscopy and Surface-Enhanced Raman Scattering. Frontiers in Chemistry, 2019, 7, 412.	3.6	32
18	Discovery of Volatile Biomarkers of Parkinson's Disease from Sebum. ACS Central Science, 2019, 5, 599-606.	11.3	100

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19	Application of HPLC–PDA–MS metabolite profiling to investigate the effect of growth temperature and day length on blackcurrant fruit. Metabolomics, 2019, 15, 12.	3.0	24
20	Rapid UHPLC-MS metabolite profiling and phenotypic assays reveal genotypic impacts of nitrogen supplementation in oats. Metabolomics, 2019, 15, 42.	3.0	16
21	Global metabolite profiles of rice brown planthopper-resistant traits reveal potential secondary metabolites for both constitutive and inducible defenses. Metabolomics, 2019, 15, 151.	3.0	13
22	Ultrasensitive Colorimetric Detection of Murine Norovirus Using NanoZyme Aptasensor. Analytical Chemistry, 2019, 91, 3270-3276.	6.5	174
23	Methodological considerations for large-scale breath analysis studies: lessons from the U-BIOPRED severe asthma project. Journal of Breath Research, 2019, 13, 016001.	3.0	20
24	On Splitting Training and Validation Set: A Comparative Study of Cross-Validation, Bootstrap and Systematic Sampling for Estimating the Generalization Performance of Supervised Learning. Journal of Analysis and Testing, 2018, 2, 249-262.	5.1	423
25	pH plays a role in the mode of action of trimethoprim on Escherichia coli. PLoS ONE, 2018, 13, e0200272.	2.5	16
26	Absolute Quantification of Uric Acid in Human Urine Using Surface Enhanced Raman Scattering with the Standard Addition Method. Analytical Chemistry, 2017, 89, 2472-2477.	6.5	112
27	Probing the action of a novel anti-leukaemic drug therapy at the single cell level using modern vibrational spectroscopy techniques. Scientific Reports, 2017, 7, 2649.	3.3	28
28	Quantitative Online Liquid Chromatography–Surface-Enhanced Raman Scattering (LC-SERS) of Methotrexate and its Major Metabolites. Analytical Chemistry, 2017, 89, 6702-6709.	6.5	63
29	Real–Time Monitoring of Enzyme–Catalysed Reactions using Deep UV Resonance Raman Spectroscopy. Chemistry - A European Journal, 2017, 23, 6983-6987.	3.3	9
30	From Multistep Enzyme Monitoring to Whole-Cell Biotransformations: Development of Real-Time Ultraviolet Resonance Raman Spectroscopy. Analytical Chemistry, 2017, 89, 12527-12532.	6.5	6
31	Through-container, extremely low concentration detection of multiple chemical markers of counterfeit alcohol using a handheld SORS device. Scientific Reports, 2017, 7, 12082.	3.3	60
32	Objective assessment of SERS thin films: comparison of silver on copper via galvanic displacement with commercially available fabricated substrates. Analytical Methods, 2017, 9, 4783-4789.	2.7	12
33	Towards improved quantitative analysis using surface-enhanced Raman scattering incorporating internal isotope labelling. Analytical Methods, 2017, 9, 6636-6644.	2.7	18
34	Metabolic Fingerprinting of Pseudomonas putida DOT-T1E Strains: Understanding the Influence of Divalent Cations in Adaptation Mechanisms Following Exposure to Toluene. Metabolites, 2016, 6, 14.	2.9	0
35	Partial Least Squares with Structured Output for Modelling the Metabolomics Data Obtained from Complex Experimental Designs: A Study into the Y-Block Coding. Metabolites, 2016, 6, 38.	2.9	9
36	Label-Free Surface Enhanced Raman Scattering Approach for High-Throughput Screening of Biocatalysts. Analytical Chemistry, 2016, 88, 5898-5903.	6.5	36

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37	Classification of Bacillus and Brevibacillus species using rapid analysis of lipids by mass spectrometry. Analytical and Bioanalytical Chemistry, 2016, 408, 7865-7878.	3.7	17
38	Rapid, Accurate, and Quantitative Detection of Propranolol in Multiple Human Biofluids via Surface-Enhanced Raman Scattering. Analytical Chemistry, 2016, 88, 10884-10892.	6.5	52
39	Rapid, accurate, and comparative differentiation of clinically and industrially relevant microorganisms via multiple vibrational spectroscopic fingerprinting. Analyst, The, 2016, 141, 5127-5136.	3.5	40
40	Rapid discrimination of Enterococcus faecium strains using phenotypic analytical techniques. Analytical Methods, 2016, 8, 7603-7613.	2.7	9
41	Intermittent energy restriction induces changes in breast gene expression and systemic metabolism. Breast Cancer Research, 2016, 18, 57.	5.0	37
42	Rapid, high-throughput, and quantitative determination of orange juice adulteration by Fourier-transform infrared spectroscopy. Analytical Methods, 2016, 8, 5581-5586.	2.7	28
43	Metabolic analysis of the response of Pseudomonas putida DOT-T1E strains to toluene using Fourier transform infrared spectroscopy and gas chromatography mass spectrometry. Metabolomics, 2016, 12, 112.	3.0	9
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. Metabolomics, 2016, 12, 82.	3.0	18
45	Metabolomic analysis of riboswitch containing E. coli recombinant expression system. Molecular BioSystems, 2016, 12, 350-361.	2.9	16
46	Metabolomics Analysis Reveals the Participation of Efflux Pumps and Ornithine in the Response of Pseudomonas putida DOT-T1E Cells to Challenge with Propranolol. PLoS ONE, 2016, 11, e0156509.	2.5	11
47	Acclimation of metabolism to light in <scp><i>A</i></scp><i>rabidopsis thaliana</i>: the glucose 6â€phosphate/phosphate translocator <scp>GPT</scp>2 directs metabolic acclimation. Plant, Cell and Environment, 2015, 38, 1404-1417.	5.7	79
48	PWE-200 Metabolomic profiling in pancreatic cancer; in search of new biomarkers. Gut, 2015, 64, A300.1-A300.	12.1	0
49	Metabolomics investigation of recombinant mTNFα production in Streptomyces lividans. Microbial Cell Factories, 2015, 14, 157.	4.0	18
50	Metabolic Profiling of Geobacter sulfurreducens during Industrial Bioprocess Scale-Up. Applied and Environmental Microbiology, 2015, 81, 3288-3298.	3.1	26
51	Surveillance for lower airway pathogens in mechanically ventilated patients by metabolomic analysis of exhaled breath: a case-control study. Thorax, 2015, 70, 320-325.	5.6	54
52	Exploring the mode of action of dithranol therapy for psoriasis: a metabolomic analysis using HaCaT cells. Molecular BioSystems, 2015, 11, 2198-2209.	2.9	20
53	PTU-093 Metabolomic profiling in inflammatory bowel disease. Gut, 2015, 64, A102.1-A102.	12.1	0
54	A tutorial review: Metabolomics and partial least squares-discriminant analysis â€" a marriage of convenience or a shotgun wedding. Analytica Chimica Acta, 2015, 879, 10-23.	5.4	618

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55	Detection and quantification of the opioid tramadol in urine using surface enhanced Raman scattering. Analyst, The, 2015, 140, 5965-5970.	3.5	34
56	Profiling of spatial metabolite distributions in wheat leaves under normal and nitrate limiting conditions. Phytochemistry, 2015, 115, 99-111.	2.9	24
57	Simultaneous multiplexed quantification of caffeine and its major metabolites theobromine and paraxanthine using surface-enhanced Raman scattering. Analytical and Bioanalytical Chemistry, 2015, 407, 8253-8261.	3.7	42
58	The influence of scaling metabolomics data on model classification accuracy. Metabolomics, 2015, 11, 684-695.	3.0	62
59	A workflow for bacterial metabolic fingerprinting and lipid profiling: application to Ciprofloxacin challenged Escherichia coli. Metabolomics, 2015, 11, 438-453.	3.0	10
60	Phenotypic Characterisation of Shewanella oneidensis MR-1 Exposed to X-Radiation. PLoS ONE, 2015, 10, e0131249.	2.5	7
61	Implementation of Fourier transform infrared spectroscopy for the rapid typing of uropathogenic Escherichia coli. European Journal of Clinical Microbiology and Infectious Diseases, 2014, 33, 983-988.	2.9	22
62	Chemometrics models for overcoming high between subject variability: applications in clinical metabolic profiling studies. Metabolomics, 2014, 10, 375-385.	3.0	12
63	A comparative investigation of modern feature selection and classification approaches for the analysis of mass spectrometry data. Analytica Chimica Acta, 2014, 829, 1-8.	5.4	93
64	Metabolomics in melon: A new opportunity for aroma analysis. Phytochemistry, 2014, 99, 61-72.	2.9	66
65	Simultaneous multiplexed quantification of nicotine and its metabolites using surface enhanced Raman scattering. Analyst, The, 2014, 139, 4820-4827.	3.5	43
66	Multiple metabolomics of uropathogenic E. coli reveal different information content in terms of metabolic potential compared to virulence factors. Analyst, The, 2014, 139, 4193-4199.	3.5	16
67	A metabolomics investigation into the effects of HIV protease inhibitors on HPV16 E6 expressing cervical carcinoma cells. Molecular BioSystems, 2014, 10, 398-411.	2.9	10
68	Compositional Equivalence of Grain from Multi-trait Drought-Tolerant Maize Hybrids to a Conventional Comparator: Univariate and Multivariate Assessments. Journal of Agricultural and Food Chemistry, 2014, 62, 9597-9608.	5.2	9
69	Optimization of matrix assisted desorption/ionization time of flight mass spectrometry (MALDI-TOF-MS) for the characterization of Bacillus and Brevibacillus species. Analytica Chimica Acta, 2014, 840, 49-57.	5.4	30
70	Influence of Missing Values Substitutes on Multivariate Analysis of Metabolomics Data. Metabolites, 2014, 4, 433-452.	2.9	158
71	Integrating multiple analytical platforms and chemometrics for comprehensive metabolic profiling: application to meat spoilage detection. Analytical and Bioanalytical Chemistry, 2013, 405, 5063-5074.	3.7	25
72	The challenge of applying Raman spectroscopy to monitor recombinant antibody production. Analyst, The, 2013, 138, 6977.	3.5	28

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73	A comparison of Raman and FT-IR spectroscopy for the prediction of meat spoilage. Food Control, 2013, 29, 461-470.	5.5	115
74	Portable, Quantitative Detection of *Bacillus* Bacterial Spores Using Surface-Enhanced Raman Scattering. Analytical Chemistry, 2013, 85, 3297-3302.	6.5	130
75	Quality Evaluation of Arnebiae Radix Using Multiple Qualitative and Quantitative Methods Coupled with Multivariate Statistical Analysis. Current Pharmaceutical Analysis, 2013, 9, 217-225.	0.6	1
76	Dupuytren's disease metabolite analyses reveals alterations following initial short-term fibroblast culturing. Molecular BioSystems, 2012, 8, 2274.	2.9	17
77	The optimisation of facile substrates for surface enhanced Raman scattering through galvanic replacement of silver onto copper. Analyst, The, 2012, 137, 2791.	3.5	27
78	Detection and Quantification of Bacterial Spoilage in Milk and Pork Meat Using MALDI-TOF-MS and Multivariate Analysis. Analytical Chemistry, 2012, 84, 5951-5958.	6.5	62
79	Multiblock principal component analysis: an efficient tool for analyzing metabolomics data which contain two influential factors. Metabolomics, 2012, 8, 37-51.	3.0	44
80	Metabolic profiling of meat: assessment of pork hygiene and contamination with Salmonella typhimurium. Analyst, The, 2011, 136, 508-514.	3.5	17
81	Fourier Transform Infrared and Raman Spectroscopies for the Rapid Detection, Enumeration, and Growth Interaction of the Bacteria Staphylococcus aureus and Lactococcus lactis ssp. cremoris in Milk. Analytical Chemistry, 2011, 83, 5681-5687.	6.5	63
82	MALDI-MS and multivariate analysis for the detection and quantification of different milk species. Analytical and Bioanalytical Chemistry, 2011, 399, 3491-3502.	3.7	72
83	Analysis of Volatile Organic Compounds in Human Saliva by a Static Sorptive Extraction Method and Gas Chromatography-Mass Spectrometry. Journal of Chemical Ecology, 2010, 36, 1035-1042.	1.8	78
84	VOC-based metabolic profiling for food spoilage detection with the application to detecting Salmonella typhimurium-contaminated pork. Analytical and Bioanalytical Chemistry, 2010, 397, 2439-2449.	3.7	50
85	Novel noninvasive identification of biomarkers by analytical profiling of chronic wounds using volatile organic compounds. Wound Repair and Regeneration, 2010, 18, 391-400.	3.0	78
86	Non-invasive metabolomic analysis of breath using differential mobility spectrometry in patients with chronic obstructive pulmonary disease and healthy smokers. Analyst, The, 2010, 135, 315.	3.5	119
87	Fourier transform infrared spectroscopy and multivariate analysis for the detection and quantification of different milk species. Journal of Dairy Science, 2010, 93, 5651-5660.	3.4	126
88	Quantitative Analysis of the Banned Food Dye Sudan-1 Using Surface Enhanced Raman Scattering with Multivariate Chemometrics. Journal of Physical Chemistry C, 2010, 114, 7285-7290.	3.1	126
89	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. Analyst, The, 2010, 135, 1235.	3.5	35
90	Assessment of adaptive focused acoustics versus manual vortex/freeze-thaw for intracellular metabolite extraction from Streptomyces lividans producing recombinant proteins using GC-MS and multi-block principal component analysis. Analyst, The, 2010, 135, 934.	3.5	25

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91	^{1}H NMR, GCâˆˆEI-TOFMS, and Data Set Correlation for Fruit Metabolomics: Application to Spatial Metabolite Analysis in Melon. Analytical Chemistry, 2009, 81, 2884-2894.	6.5	147
92	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. Analyst, The, 2009, 134, 114-123.	3.5	39
93	Individual and gender fingerprints in human body odour. Journal of the Royal Society Interface, 2007, 4, 331-340.	3.4	320
94	Application of Dissimilarity Indices, Principal Coordinates Analysis, and Rank Tests to Peak Tables in Metabolomics of the Gas Chromatography/Mass Spectrometry of Human Sweat. Analytical Chemistry, 2007, 79, 5633-5641.	6.5	37
95	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. Analyst, The, 2007, 132, 638.	3.5	7
96	Pattern recognition of gas chromatography mass spectrometry of human volatiles in sweat to distinguish the sex of subjects and determine potential discriminatory marker peaks. Chemometrics and Intelligent Laboratory Systems, 2007, 87, 161-172.	3.5	64
97	Automated single-nucleotide polymorphism analysis using fluorescence excitationâ€"emission spectroscopy and one-class classifiers. Analytical and Bioanalytical Chemistry, 2007, 388, 655-664.	3.7	2
98	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. Metabolomics, 2007, 3, 427-437.	3.0	43
99	Support Vector Machines: A Recent Method for Classification in Chemometrics. Critical Reviews in Analytical Chemistry, 2006, 36, 177-188.	3.5	152
100	A comparative study of cluster validation indices applied to genotyping data. Chemometrics and Intelligent Laboratory Systems, 2005, 78, 30-40.	3.5	19
101	Diagnostic Pattern Recognition on Gene-Expression Profile Data by Using One-Class Classification. Journal of Chemical Information and Modeling, 2005, 45, 1392-1401.	5.4	15