Roy Goodacre

List of Publications by Year
in descending order

478 papers	40,480 citations	2669 95 h-index	3476 182 g-index
496 all docs	496 docs citations	496 times ranked	40316 citing authors

#	Article	IF	Citations
1	Proposed minimum reporting standards for chemical analysis. Metabolomics, 2007, 3, 211-221.	1.4	3,589
2	Procedures for large-scale metabolic profiling of serum and plasma using gas chromatography and liquid chromatography coupled to mass spectrometry. Nature Protocols, 2011, 6, 1060-1083.	5.5	2,236
3	Present and Future of Surface-Enhanced Raman Scattering. ACS Nano, 2020, 14, 28-117.	7.3	2,153
4	Metabolomics by numbers: acquiring and understanding global metabolite data. Trends in Biotechnology, 2004, 22, 245-252.	4.9	1,156
5	Identification of Novel Genes in Arabidopsis Involved in Secondary Cell Wall Formation Using Expression Profiling and Reverse Genetics. Plant Cell, 2005, 17, 2281-2295.	3.1	715
6	Systems level studies of mammalian metabolomes: the roles of mass spectrometry and nuclear magnetic resonance spectroscopy. Chemical Society Reviews, 2011, 40, 387-426.	18.7	689
7	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.	2.6	618
8	Discrimination of Bacteria Using Surface-Enhanced Raman Spectroscopy. Analytical Chemistry, 2004, 76, 40-47.	3.2	608
9	Metabolic fingerprinting in disease diagnosis: biomedical applications of infrared and Raman spectroscopy. Analyst, The, 2006, 131, 875.	1.7	544
10	Guidelines and considerations for the use of system suitability and quality control samples in mass spectrometry assays applied in untargeted clinical metabolomic studies. Metabolomics, 2018, 14, 72.	1.4	517
11	Metabolomics: Current technologies and future trends. Proteomics, 2006, 6, 4716-4723.	1.3	471
12	Mass appeal: metabolite identification in mass spectrometry-focused untargeted metabolomics. Metabolomics, 2013, 9, 44-66.	1.4	452
13	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.	2.5	423
14	The metabolomics standards initiative (MSI). Metabolomics, 2007, 3, 175-178.	1.4	396
15	Fingerprinting food: current technologies for the detection of food adulteration and contamination. Chemical Society Reviews, 2012, 41, 5706.	18.7	362
16	Rapid identification of urinary tract infection bacteria using hyperspectral whole-organism fingerprinting and artificial neural networks. Microbiology (United Kingdom), 1998, 144, 1157-1170.	0.7	361
17	Metabolic fingerprinting as a diagnostic tool. Pharmacogenomics, 2007, 8, 1243-1266.	0.6	361
18	Proposed minimum reporting standards for data analysis in metabolomics. Metabolomics, 2007, 3, 231-241.	1.4	361

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19	Characterisation and identification of bacteria using SERS. Chemical Society Reviews, 2008, 37, 931.	18.7	352
20	Comparison of five xylan synthesis mutants reveals new insight into the mechanisms of xylan synthesis. Plant Journal, 2007, 52, 1154-1168.	2.8	338
21	The role of reporting standards for metabolite annotation and identification in metabolomic studies. GigaScience, 2013, 2, 13.	3.3	333
22	The Metabolomics Standards Initiative. Nature Biotechnology, 2007, 25, 846-848.	9.4	328
23	Global Metabolic Profiling of <i>Escherichia coli</i> Cultures:â€‰ an Evaluation of Methods for Quenching and Extraction of Intracellular Metabolites. Analytical Chemistry, 2008, 80, 2939-2948.	3.2	293
24	Detection of the Dipicolinic Acid Biomarker inBacillusSpores Using Curie-Point Pyrolysis Mass Spectrometry and Fourier Transform Infrared Spectroscopy. Analytical Chemistry, 2000, 72, 119-127.	3.2	292
25	The role of metabolites and metabolomics in clinically applicable biomarkers of disease. Archives of Toxicology, 2011, 85, 5-17.	1.9	289
26	A proposed framework for the description of plant metabolomics experiments and their results. Nature Biotechnology, 2004, 22, 1601-1606.	9.4	283
27	Rapid and Quantitative Detection of the Microbial Spoilage of Meat by Fourier Transform Infrared Spectroscopy and Machine Learning. Applied and Environmental Microbiology, 2002, 68, 2822-2828.	1.4	281
28	Genetic algorithms as a method for variable selection in multiple linear regression and partial least squares regression, with applications to pyrolysis mass spectrometry. Analytica Chimica Acta, 1997, 348, 71-86.	2.6	259
29	Mass spectrometry tools and metabolite-specific databases for molecular identification in metabolomics. Analyst, The, 2009, 134, 1322.	1.7	240
30	Surface-Enhanced Raman Spectroscopy for Bacterial Discrimination Utilizing a Scanning Electron Microscope with a Raman Spectroscopy Interface. Analytical Chemistry, 2004, 76, 5198-5202.	3.2	231
31	Surface-enhanced Raman scattering for the rapid discrimination of bacteria. Faraday Discussions, 2006, 132, 281-292.	1.6	222
32	Metabolomics of a Superorganism. Journal of Nutrition, 2007, 137, 259S-266S.	1.3	220
33	Metabolic fingerprinting of salt-stressed tomatoes. Phytochemistry, 2003, 62, 919-928.	1.4	210
34	An introduction to liquid chromatographyâ€"mass spectrometry instrumentation applied in plant metabolomic analyses. Phytochemical Analysis, 2010, 21, 33-47.	1.2	207
35	Molecular phenotyping of a UK population: defining the human serum metabolome. Metabolomics, 2015, 11, 9-26.	1.4	202
36	Metabolomic technologies and their application to the study of plants and plantâ€"host interactions. Physiologia Plantarum, 2008, 132, 117-135.	2.6	201

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37	New cofactor supports Î±,Î²-unsaturated acid decarboxylation via 1,3-dipolar cycloaddition. Nature, 2015, 522, 497-501.	13.7	197
38	Rapid identification of Streptococcus and Enterococcus species using diffuse reflectance-absorbance Fourier transform infrared spectroscopy and artificial neural networks. FEMS Microbiology Letters, 1996, 140, 233-239.	0.7	187
39	Metabolite extraction from suspension-cultured mammalian cells for global metabolite profiling. Nature Protocols, 2011, 6, 1241-1249.	5.5	186
40	Rapid and quantitative detection of the microbial spoilage of muscle foods: current status and future trends. Trends in Food Science and Technology, 2001, 12, 414-424.	7.8	185
41	Shining Light on the Microbial World. Advances in Applied Microbiology, 2010, 70, 153-186.	1.3	185
42	Point-and-shoot: rapid quantitative detection methods for on-site food fraud analysis â€" moving out of the laboratory and into the food supply chain. Analytical Methods, 2015, 7, 9401-9414.	1.3	183
43	Rapid Differentiation of Closely Related <i>Candida</i> Species and Strains by Pyrolysis-Mass Spectrometry and Fourier Transform-Infrared Spectroscopy. Journal of Clinical Microbiology, 1998, 36, 367-374.	1.8	181
44	Exhaled breath analysis: a review of â€˜breath-takingâ€™ methods for off-line analysis. Metabolomics, 2017, 13, 110.	1.4	178
45	Ultrasensitive Colorimetric Detection of Murine Norovirus Using NanoZyme Aptasensor. Analytical Chemistry, 2019, 91, 3270-3276.	3.2	174
46	Automated workflows for accurate mass-based putative metabolite identification in LC/MS-derived metabolomic datasets. Bioinformatics, 2011, 27, 1108-1112.	1.8	173
47	SERS Detection of Multiple Antimicrobial-Resistant Pathogens Using Nanosensors. Analytical Chemistry, 2017, 89, 12666-12673.	3.2	170
48	Development and Performance of a Gas Chromatographyâˆ'Time-of-Flight Mass Spectrometry Analysis for Large-Scale Nontargeted Metabolomic Studies of Human Serum. Analytical Chemistry, 2009, 81, 7038-7046.	3.2	168
49	UbiX is a flavin prenyltransferase required for bacterial ubiquinone biosynthesis. Nature, 2015, 522, 502-506.	13.7	168
50	Systems biology guided by XCMS Online metabolomics. Nature Methods, 2017, 14, 461-462.	9.0	168
51	Illuminating disease and enlightening biomedicine: Raman spectroscopy as a diagnostic tool. Analyst, The, 2013, 138, 3871.	1.7	163
52	Clinical applications of infrared and Raman spectroscopy: state of play and future challenges. Analyst, The, 2018, 143, 1735-1757.	1.7	163
53	An automated Design-Build-Test-Learn pipeline for enhanced microbial production of fine chemicals. Communications Biology, 2018, 1, 66.	2.0	159
54	Influence of Missing Values Substitutes on Multivariate Analysis of Metabolomics Data. Metabolites, 2014, 4, 433-452.	1.3	158

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55	Rapid Quantitative Assessment of the Adulteration of Virgin Olive Oils with Hazelnut Oils Using Raman Spectroscopy and Chemometrics. Journal of Agricultural and Food Chemistry, 2003, 51, 6145-6150.	2.4	153
56	A metabolome pipeline: from concept to data to knowledge. Metabolomics, 2005, 1, 39-51.	1.4	152
57	Genetic algorithm optimization for pre-processing and variable selection of spectroscopic data. Bioinformatics, 2005, 21, 860-868.	1.8	149
58	¹H NMR, GCâˆ’EI-TOFMS, and Data Set Correlation for Fruit Metabolomics: Application to Spatial Metabolite Analysis in Melon. Analytical Chemistry, 2009, 81, 2884-2894.	3.2	147
59	Metabolomics and systems pharmacology: why and how to model the human metabolic network for drug discovery. Drug Discovery Today, 2014, 19, 171-182.	3.2	140
60	COordination of Standards in MetabOlomicS (COSMOS): facilitating integrated metabolomics data access. Metabolomics, 2015, 11, 1587-1597.	1.4	140
61	Chemical and bioanalytical applications of surface enhanced Raman scattering spectroscopy. Chemical Society Reviews, 2008, 37, 883.	18.7	136
62	Metabolomic analysis of the interaction between plants and herbivores. Metabolomics, 2009, 5, 150-161.	1.4	135
63	Simultaneous detection and quantification of three bacterial meningitis pathogens by SERS. Chemical Science, 2014, 5, 1030-1040.	3.7	134
64	Effective Quenching Processes for Physiologically Valid Metabolite Profiling of Suspension Cultured Mammalian Cells. Analytical Chemistry, 2009, 81, 174-183.	3.2	132
65	Taking your breath away: metabolomics breathes life in to personalized medicine. Trends in Biotechnology, 2014, 32, 538-548.	4.9	132
66	Characterization of Microorganisms Using UV Resonance Raman Spectroscopy and Chemometrics. Analytical Chemistry, 2004, 76, 585-591.	3.2	131
67	Portable, Quantitative Detection of <i>Bacillus</i> Bacterial Spores Using Surface-Enhanced Raman Scattering. Analytical Chemistry, 2013, 85, 3297-3302.	3.2	130
68	Metabolic profiling using direct infusion electrospray ionisation mass spectrometry for the characterisation of olive oils. Analyst, The, 2002, 127, 1457-1462.	1.7	127
69	Recent developments in quantitative SERS: Moving towards absolute quantification. TrAC - Trends in Analytical Chemistry, 2018, 102, 359-368.	5.8	127
70	Chemometric discrimination of unfractionated plant extracts analyzed by electrospray mass spectrometry. Phytochemistry, 2003, 62, 859-863.	1.4	126
71	Multiplexed detection of six labelled oligonucleotides using surface enhanced resonance Raman scattering (SERRS). Analyst, The, 2008, 133, 1505.	1.7	126
72	Fourier transform infrared spectroscopy and multivariate analysis for the detection and quantification of different milk species. Journal of Dairy Science, 2010, 93, 5651-5660.	1.4	126

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73	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.	1.5	126
74	Flow infusion electrospray ionisation mass spectrometry for high throughput, non-targeted metabolite fingerprinting: a review. Metabolomics, 2013, 9, 4-29.	1.4	124
75	Rapid assessment of the adulteration of virgin olive oils by other seed oils using pyrolysis mass spectrometry and artificial neural networks. Journal of the Science of Food and Agriculture, 1993, 63, 297-307.	1.7	120
76	Progress toward the Rapid Nondestructive Assessment of the Floral Origin of European Honey Using Dispersive Raman Spectroscopy. Applied Spectroscopy, 2002, 56, 521-527.	1.2	120
77	Inter-laboratory reproducibility of fast gas chromatographyâ€“electron impactâ€“time of flight mass spectrometry (GCâ€“EIâ€“TOF/MS) based plant metabolomics. Metabolomics, 2009, 5, 479-496.	1.4	120
78	Rapid and quantitative detection of the microbial spoilage of beef by Fourier transform infrared spectroscopy and machine learning. Analytica Chimica Acta, 2004, 514, 193-201.	2.6	119
79	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.	1.7	119
80	Is Serum or Plasma More Appropriate for Intersubject Comparisons in Metabolomic Studies? An Assessment in Patients with Small-Cell Lung Cancer. Analytical Chemistry, 2011, 83, 6689-6697.	3.2	119
81	Electronic cigarette exposure triggers neutrophil inflammatory responses. Respiratory Research, 2016, 17, 56.	1.4	117
82	Metabolomic approaches reveal that phosphatidic and phosphatidyl glycerol phospholipids are major discriminatory nonâ€polar metabolites in responses by Brachypodium distachyon to challenge by Magnaporthe grisea. Plant Journal, 2006, 46, 351-368.	2.8	115
83	A comparison of Raman and FT-IR spectroscopy for the prediction of meat spoilage. Food Control, 2013, 29, 461-470.	2.8	115
84	Surface-Enhanced Raman Scattering from Intracellular and Extracellular Bacterial Locations. Analytical Chemistry, 2008, 80, 6741-6746.	3.2	114
85	Untargeted Metabolic Profiling Identifies Altered Serum Metabolites of Type 2 Diabetes Mellitus in a Prospective, Nested Case Control Study. Clinical Chemistry, 2015, 61, 487-497.	1.5	113
86	Pyrolysis mass spectrometry and its applications in biotechnology. Current Opinion in Biotechnology, 1996, 7, 20-28.	3.3	112
87	Absolute Quantification of Uric Acid in Human Urine Using Surface Enhanced Raman Scattering with the Standard Addition Method. Analytical Chemistry, 2017, 89, 2472-2477.	3.2	112
88	Extensive metabolic crossâ€talk in melon fruit revealed by spatial and developmental combinatorial metabolomics. New Phytologist, 2011, 190, 683-696.	3.5	111
89	Functional Genomics via Metabolic Footprinting: Monitoring Metabolite Secretion byEscherichia coliTryptophan Metabolism Mutants Using FTâ€“IR and Direct Injection Electrospray Mass Spectrometry. Comparative and Functional Genomics, 2003, 4, 376-391.	2.0	110
90	Metabolite profiling of recombinant CHO cells: Designing tailored feeding regimes that enhance recombinant antibody production. Biotechnology and Bioengineering, 2011, 108, 3025-3031.	1.7	110

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91	Variable Selection in Discriminant Partial Least-Squares Analysis. Analytical Chemistry, 1998, 70, 4126-4133.	3.2	109
92	Rapid identification of closely related muscle foods by vibrational spectroscopy and machine learning. Analyst, The, 2005, 130, 1648.	1.7	109
93	Meat, the metabolites: an integrated metabolite profiling and lipidomics approach for the detection of the adulteration of beef with pork. Analyst, The, 2016, 141, 2155-2164.	1.7	106
94	Raman Activated Cell Ejection for Isolation of Single Cells. Analytical Chemistry, 2013, 85, 10697-10701.	3.2	105
95	Metabolic footprinting as a tool for discriminating between brewing yeasts. Yeast, 2007, 24, 667-679.	0.8	103
96	Discovery of Volatile Biomarkers of Parkinsonâ€™s Disease from Sebum. ACS Central Science, 2019, 5, 599-606.	5.3	100
97	Metabolomics for the masses: The future of metabolomics in a personalized world. European Journal of Molecular and Clinical Medicine, 2017, 3, 294.	0.5	99
98	Rapid and quantitative detection of the microbial spoilage in milk using Fourier transform infrared spectroscopy and chemometrics. Analyst, The, 2008, 133, 1424.	1.7	98
99	Flow-injection electrospray ionization mass spectrometry of crude cell extracts for high-throughput bacterial identification. Journal of the American Society for Mass Spectrometry, 2002, 13, 118-128.	1.2	97
100	Data standards can boost metabolomics research, and if there is a will, there is a way. Metabolomics, 2016, 12, 14.	1.4	97
101	Exhaled Volatile Organic Compounds of Infection: A Systematic Review. ACS Infectious Diseases, 2017, 3, 695-710.	1.8	96
102	Rapid and Quantitative Analysis of the Pyrolysis Mass Spectra of Complex Binary and Tertiary Mixtures Using Multivariate Calibration and Artificial Neural Networks. Analytical Chemistry, 1994, 66, 1070-1085.	3.2	94
103	Ultra-violet resonance Raman spectroscopy for the rapid discrimination of urinary tract infection bacteria. FEMS Microbiology Letters, 2004, 232, 127-132.	0.7	94
104	Discrimination of Aerobic Endospore-forming Bacteria via Electrospray-Ionization Mass Spectrometry of Whole Cell Suspensions. Analytical Chemistry, 2001, 73, 4134-4144.	3.2	93
105	A comparative investigation of modern feature selection and classification approaches for the analysis of mass spectrometry data. Analytica Chimica Acta, 2014, 829, 1-8.	2.6	93
106	Rapid identification using pyrolysis mass spectrometry and artificial neural networks of <i>Propionibacterium acnes</i> isolated from dogs. Journal of Applied Bacteriology, 1994, 76, 124-134.	1.1	91
107	Metabolomics of sebum reveals lipid dysregulation in Parkinsonâ€™s disease. Nature Communications, 2021, 12, 1592.	5.8	91
108	Evaluation of extraction processes for intracellular metabolite profiling of mammalian cells: matching extraction approaches to cell type and metabolite targets. Metabolomics, 2010, 6, 427-438.	1.4	88

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109	Dual metabolomics: A novel approach to understanding plantâ€“pathogen interactions. Phytochemistry, 2010, 71, 590-597.	1.4	88
110	Rapid monitoring of antibiotics using Raman and surface enhanced Raman spectroscopy. Analyst, The, 2005, 130, 1019.	1.7	85
111	Monitoring the Mode of Action of Antibiotics Using Raman Spectroscopy:Â Investigating Subinhibitory Effects of Amikacin onPseudomonasaeruginosa. Analytical Chemistry, 2005, 77, 2901-2906.	3.2	84
112	Neural networks and olive oil. Nature, 1992, 359, 594-594.	13.7	83
113	Diffuse reflectance absorbance spectroscopy taking in chemometrics (DRASTIC). A hyperspectral FT-IR-based approach to rapid screening for metabolite overproduction. Analytica Chimica Acta, 1997, 348, 273-282.	2.6	82
114	Explanatory analysis of spectroscopic data using machine learning of simple, interpretable rules. Vibrational Spectroscopy, 2003, 32, 33-45.	1.2	82
115	Accumulation of ionic liquids in Escherichia coli cells. Green Chemistry, 2008, 10, 836.	4.6	82
116	Noninvasive, On-Line Monitoring of the Biotransformation by Yeast of Glucose to Ethanol Using Dispersive Raman Spectroscopy and Chemometrics. Applied Spectroscopy, 1999, 53, 1419-1428.	1.2	81
117	Monitoring of complex industrial bioprocesses for metabolite concentrations using modern spectroscopies and machine learning: Application to gibberellic acid production. Biotechnology and Bioengineering, 2002, 78, 527-538.	1.7	79
118	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.	2.8	79
119	Root functional traits explain root exudation rate and composition across a range of grassland species. Journal of Ecology, 2022, 110, 21-33.	1.9	79
120	Novel noninvasive identification of biomarkers by analytical profiling of chronic wounds using volatile organic compounds. Wound Repair and Regeneration, 2010, 18, 391-400.	1.5	78
121	Plant Metabolomics and Its Potential for Systems Biology Research. Methods in Enzymology, 2011, 500, 299-336.	0.4	78
122	Combining Raman and FT-IR Spectroscopy with Quantitative Isotopic Labeling for Differentiation of <i>E. coli</i> Cells at Community and Single Cell Levels. Analytical Chemistry, 2015, 87, 4578-4586.	3.2	78
123	Metabolomic approaches reveal that cell wall modifications play a major role in ethyleneâ€mediated resistance against <i>Botrytis cinerea</i>. Plant Journal, 2011, 67, 852-868.	2.8	77
124	Classification of pyrolysis mass spectra by fuzzy multivariate rule induction-comparison with regression, K-nearest neighbour, neural and decision-tree methods. Analytica Chimica Acta, 1997, 348, 389-407.	2.6	75
125	PYCHEM: a multivariate analysis package for python. Bioinformatics, 2006, 22, 2565-2566.	1.8	75
126	Metabolic acclimation to hypoxia revealed by metabolite gradients in melon fruit. Journal of Plant Physiology, 2010, 167, 242-245.	1.6	75

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127	Metabolic responses of eukaryotic microalgae to environmental stress limit the ability of FT-IR spectroscopy for species identification. Algal Research, 2015, 11, 148-155.	2.4	74
128	Application of high-throughput Fourier-transform infrared spectroscopy in toxicology studies: contribution to a study on the development of an animal model for idiosyncratic toxicity. Toxicology Letters, 2004, 146, 197-205.	0.4	73
129	MALDI-MS and multivariate analysis for the detection and quantification of different milk species. Analytical and Bioanalytical Chemistry, 2011, 399, 3491-3502.	1.9	72
130	Reverse and Multiple Stable Isotope Probing to Study Bacterial Metabolism and Interactions at the Single Cell Level. Analytical Chemistry, 2016, 88, 9443-9450.	3.2	72
131	Investigating plantâ€“plant interference by metabolic fingerprinting. Phytochemistry, 2003, 63, 705-710.	1.4	71
132	Rapid identification of species within the Mycobacterium tuberculosis complex by artificial neural network analysis of pyrolysis mass spectra. Journal of Medical Microbiology, 1994, 40, 170-173.	0.7	70
133	Metabolic dysregulation in vitaminÂE and carnitine shuttle energy mechanisms associate with human frailty. Nature Communications, 2019, 10, 5027.	5.8	70
134	Computational tools and workflows in metabolomics: An international survey highlights the opportunity for harmonisation through Galaxy. Metabolomics, 2017, 13, 12.	1.4	69
135	Screening ionic liquids for use in biotransformations with whole microbial cells. Green Chemistry, 2011, 13, 1843.	4.6	68
136	Correction of Mass Spectral Drift Using Artificial Neural Networks. Analytical Chemistry, 1996, 68, 271-280.	3.2	67
137	Making sense of the metabolome using evolutionary computation: seeing the wood with the trees. Journal of Experimental Botany, 2004, 56, 245-254.	2.4	66
138	Metabolomics in melon: A new opportunity for aroma analysis. Phytochemistry, 2014, 99, 61-72.	1.4	66
139	Optimization of Parameters for the Quantitative Surface-Enhanced Raman Scattering Detection of Mephedrone Using a Fractional Factorial Design and a Portable Raman Spectrometer. Analytical Chemistry, 2013, 85, 923-931.	3.2	65
140	A novel untargeted metabolomics correlation-based network analysis incorporating human metabolic reconstructions. BMC Systems Biology, 2013, 7, 107.	3.0	64
141	Rapid and quantitative analysis and bioprocesses using pyrolysis mass spectrometry and neural networks: application to indole production. Analytica Chimica Acta, 1993, 279, 17-26.	2.6	63
142	Matrix-suppressed laser desorption/ionisation mass spectrometry and its suitability for metabolome analyses. Rapid Communications in Mass Spectrometry, 2006, 20, 1192-1198.	0.7	63
143	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.	3.2	63
144	A comparison of different chemometrics approaches for the robust classification of electronic nose data. Analytical and Bioanalytical Chemistry, 2014, 406, 7581-7590.	1.9	63

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145	Quantitative Online Liquid Chromatographyâ€“Surface-Enhanced Raman Scattering (LC-SERS) of Methotrexate and its Major Metabolites. Analytical Chemistry, 2017, 89, 6702-6709.	3.2	63
146	Using a biphasic ionic liquid/water reaction system to improve oxygenase-catalysed biotransformation with whole cells. Green Chemistry, 2008, 10, 685.	4.6	62
147	Detection and Quantification of Bacterial Spoilage in Milk and Pork Meat Using MALDI-TOF-MS and Multivariate Analysis. Analytical Chemistry, 2012, 84, 5951-5958.	3.2	62
148	The influence of scaling metabolomics data on model classification accuracy. Metabolomics, 2015, 11, 684-695.	1.4	62
149	Subsurface Biomolecular Imaging of <i>Streptomyces </i><i>coelicolor</i> Using Secondary Ion Mass Spectrometry. Analytical Chemistry, 2008, 80, 1942-1951.	3.2	61
150	Characterisation of intact microorganisms using electrospray ionisation mass spectrometry. FEMS Microbiology Letters, 1999, 176, 17-24.	0.7	60
151	Raman spectroscopy: lighting up the future of microbial identification. Future Microbiology, 2011, 6, 991-997.	1.0	60
152	Through-container, extremely low concentration detection of multiple chemical markers of counterfeit alcohol using a handheld SORS device. Scientific Reports, 2017, 7, 12082.	1.6	60
153	Untargeted metabolomics of COVID-19 patient serum reveals potential prognostic markers of both severity and outcome. Metabolomics, 2022, 18, 6.	1.4	60
154	Metabolic fingerprints of Mycobacterium bovis cluster with molecular type: implications for genotypeâ€“phenotype links. Microbiology (United Kingdom), 2006, 152, 2757-2765.	0.7	58
155	A flavour of omics approaches for the detection of food fraud. Current Opinion in Food Science, 2016, 10, 7-15.	4.1	58
156	Metabolomics-assisted synthetic biology. Current Opinion in Biotechnology, 2012, 23, 22-28.	3.3	56
157	Comparison of diffuse-reflectance absorbance and attenuated total reflectance FT-IR for the discrimination of bacteria. Analyst, The, 2004, 129, 1118.	1.7	55
158	Surveillance for lower airway pathogens in mechanically ventilated patients by metabolomic analysis of exhaled breath: a case-control study. Thorax, 2015, 70, 320-325.	2.7	54
159	Surface-Enhanced Raman Scattering (SERS) in Microbiology: Illumination and Enhancement of the Microbial World. Applied Spectroscopy, 2018, 72, 987-1000.	1.2	54
160	Genetic Programming:Â A Novel Method for the Quantitative Analysis of Pyrolysis Mass Spectral Data. Analytical Chemistry, 1997, 69, 4381-4389.	3.2	53
161	Sample preparation in matrix-assisted laser desorption/ionization mass spectrometry of whole bacterial cells and the detection of high mass (>20?kDa) proteins. Rapid Communications in Mass Spectrometry, 2002, 16, 1276-1286.	0.7	53
162	Integration of metabolomics in heart disease and diabetes research: current achievements and future outlook. Bioanalysis, 2011, 3, 2205-2222.	0.6	53

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163	Rapid, Accurate, and Quantitative Detection of Propranolol in Multiple Human Biofluids via Surface-Enhanced Raman Scattering. Analytical Chemistry, 2016, 88, 10884-10892.	3.2	52
164	Rapid screening for metabolite overproduction in fermentor broths, using pyrolysis mass spectrometry with multivariate calibration and artificial neural networks. Biotechnology and Bioengineering, 1994, 44, 1205-1216.	1.7	51
165	Quantitative Analysis of Multivariate Data Using Artificial Neural Networks: A Tutorial Review and Applications to the Deconvolution of Pyrolysis Mass Spectra. Zentralblatt Fur Bakteriologie: International Journal of Medical Microbiology, 1996, 284, 516-539.	0.5	50
166	On mass spectrometer instrument standardization and interlaboratory calibration transfer using neural networks. Analytica Chimica Acta, 1997, 348, 511-532.	2.6	50
167	Predicting human embryo viability: the road to non-invasive analysis of the secretome using metabolic footprinting. Reproductive BioMedicine Online, 2007, 15, 296-302.	1.1	50
168	Relatedness of medically important strains of <i>Saccharomyces cerevisiae</i> as revealed by phylogenetics and metabolomics. Yeast, 2008, 25, 501-512.	0.8	50
169	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.	1.9	50
170	Rapid monitoring of recombinant antibody production by mammalian cell cultures using fourier transform infrared spectroscopy and chemometrics. Biotechnology and Bioengineering, 2010, 106, 432-442.	1.7	50
171	Monitoring the Glycosylation Status of Proteins Using Raman Spectroscopy. Analytical Chemistry, 2011, 83, 6074-6081.	3.2	50
172	Enhancing Disease Diagnosis: Biomedical Applications of Surface-Enhanced Raman Scattering. Applied Sciences (Switzerland), 2019, 9, 1163.	1.3	50
173	Surface Enhanced Raman Spectroscopy for Quantitative Analysis: Results of a Large-Scale European Multi-Instrument Interlaboratory Study. Analytical Chemistry, 2020, 92, 4053-4064.	3.2	50
174	Increased intracellular proteolysis reduces disease severity in an ER stressâ€“associated dwarfism. Journal of Clinical Investigation, 2017, 127, 3861-3865.	3.9	50
175	Rapid and quantitative analysis of metabolites in fermentor broths using pyrolysis mass spectrometry with supervised learning: application to the screening of Penicillium chrysogenum fermentations for the overproduction of penicillins. Analytica Chimica Acta, 1995, 313, 25-43.	2.6	49
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