Roy Goodacre

List of Publications by Citations

453 papers	31,037 citations	88 h-index	161 g-index
495 ext. papers	36,209 ext. citations	6.4 avg, IF	7.28 L-index

#	Paper	IF	Citations
453	Proposed minimum reporting standards for chemical analysis Chemical Analysis Working Group (CAWG) Metabolomics Standards Initiative (MSI). *Metabolomics*, **2007**, 3, 211-221	4.7	2472
452	Procedures for large-scale metabolic profiling of serum and plasma using gas chromatography and liquid chromatography coupled to mass spectrometry. *Nature Protocols*, **2011**, 6, 1060-83	18.8	1527
451	Metabolomics by numbers: acquiring and understanding global metabolite data. *Trends in Biotechnology*, **2004**, 22, 245-52	15.1	1001
450	Present and Future of Surface-Enhanced Raman Scattering. *ACS Nano*, **2020**, 14, 28-117	16.7	1000
449	Identification of novel genes in Arabidopsis involved in secondary cell wall formation using expression profiling and reverse genetics. *Plant Cell*, **2005**, 17, 2281-95	11.6	598
448	Systems level studies of mammalian metabolomes: the roles of mass spectrometry and nuclear magnetic resonance spectroscopy. *Chemical Society Reviews*, **2011**, 40, 387-426	58.5	565
447	Discrimination of bacteria using surface-enhanced Raman spectroscopy. *Analytical Chemistry*, **2004**, 76, 40-7	7.8	528
446	A tutorial review: Metabolomics and partial least squares-discriminant analysis--a marriage of convenience or a shotgun wedding. *Analytica Chimica Acta*, **2015**, 879, 10-23	6.6	478
445	Metabolic fingerprinting in disease diagnosis: biomedical applications of infrared and Raman spectroscopy. *Analyst, The*, **2006**, 131, 875-85	5	458
444	Metabolomics: current technologies and future trends. *Proteomics*, **2006**, 6, 4716-23	4.8	402
443	Mass appeal: metabolite identification in mass spectrometry-focused untargeted metabolomics. *Metabolomics*, **2013**, 9, 44-66	4.7	369
442	Rapid identification of urinary tract infection bacteria using hyperspectral whole-organism fingerprinting and artificial neural networks. *Microbiology (United Kingdom)*, **1998**, 144 (Pt 5), 1157-1170	2.9	324
441	Proposed minimum reporting standards for data analysis in metabolomics. *Metabolomics*, **2007**, 3, 231-241	4.7	317
440	Metabolic fingerprinting as a diagnostic tool. *Pharmacogenomics*, **2007**, 8, 1243-66	2.6	313
439	Characterisation and identification of bacteria using SERS. *Chemical Society Reviews*, **2008**, 37, 931-6	58.5	307
438	The metabolomics standards initiative (MSI). *Metabolomics*, **2007**, 3, 175-178	4.7	304
437	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	4.7	303

436	Fingerprinting food: current technologies for the detection of food adulteration and contamination. *Chemical Society Reviews*, **2012**, 41, 5706-27	58.5	283
435	Comparison of five xylan synthesis mutants reveals new insight into the mechanisms of xylan synthesis. *Plant Journal*, **2007**, 52, 1154-68	6.9	271
434	A proposed framework for the description of plant metabolomics experiments and their results. *Nature Biotechnology*, **2004**, 22, 1601-6	44.5	260
433	Detection of the dipicolinic acid biomarker in Bacillus spores using Curie-point pyrolysis mass spectrometry and Fourier transform infrared spectroscopy. *Analytical Chemistry*, **2000**, 72, 119-27	7.8	256
432	The metabolomics standards initiative. *Nature Biotechnology*, **2007**, 25, 846-8	44.5	253
431	Global metabolic profiling of Escherichia coli cultures: an evaluation of methods for quenching and extraction of intracellular metabolites. *Analytical Chemistry*, **2008**, 80, 2939-48	7.8	251
430	Rapid and quantitative detection of the microbial spoilage of meat by fourier transform infrared spectroscopy and machine learning. *Applied and Environmental Microbiology*, **2002**, 68, 2822-8	4.8	240
429	The role of metabolites and metabolomics in clinically applicable biomarkers of disease. *Archives of Toxicology*, **2011**, 85, 5-17	5.8	233
428	Mass spectrometry tools and metabolite-specific databases for molecular identification in metabolomics. *Analyst, The*, **2009**, 134, 1322-32	5	215
427	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	6.6	215
426	Surface-enhanced Raman spectroscopy for bacterial discrimination utilizing a scanning electron microscope with a Raman spectroscopy interface. *Analytical Chemistry*, **2004**, 76, 5198-202	7.8	201
425	Surface-enhanced Raman scattering for the rapid discrimination of bacteria. *Faraday Discussions*, **2006**, 132, 281-92; discussion 309-19	3.6	196
424	Metabolic fingerprinting of salt-stressed tomatoes. *Phytochemistry*, **2003**, 62, 919-28	4	194
423	Metabolomics of a superorganism. *Journal of Nutrition*, **2007**, 137, 259S-266S	4.1	188
422	An introduction to liquid chromatography-mass spectrometry instrumentation applied in plant metabolomic analyses. *Phytochemical Analysis*, **2010**, 21, 33-47	3.4	182
421	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	2.9	179
420	Molecular phenotyping of a UK population: defining the human serum metabolome. *Metabolomics*, **2015**, 11, 9-26	4.7	167
419	Metabolomic technologies and their application to the study of plants and plant-host interactions. *Physiologia Plantarum*, **2008**, 132, 117-35	4.6	165

418	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	3.2	160
417	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	15.3	159
416	New cofactor supports [illegible]unsaturated acid decarboxylation via 1,3-dipolar cycloaddition. *Nature*, **2015**, 522, 497-501	50.4	156
415	Automated workflows for accurate mass-based putative metabolite identification in LC/MS-derived metabolomic datasets. *Bioinformatics*, **2011**, 27, 1108-12	7.2	156
414	Development and performance of a gas chromatography-time-of-flight mass spectrometry analysis for large-scale nontargeted metabolomic studies of human serum. *Analytical Chemistry*, **2009**, 81, 7038-46	7.8	152
413	Point-and-shoot: rapid quantitative detection methods for on-site food fraud analysis [illegible]moving out of the laboratory and into the food supply chain. *Analytical Methods*, **2015**, 7, 9401-9414	3.2	149
412	Rapid differentiation of closely related Candida species and strains by pyrolysis-mass spectrometry and Fourier transform-infrared spectroscopy. *Journal of Clinical Microbiology*, **1998**, 36, 367-74	9.7	143
411	Metabolite extraction from suspension-cultured mammalian cells for global metabolite profiling. *Nature Protocols*, **2011**, 6, 1241-9	18.8	142
410	Shining light on the microbial world the application of Raman microspectroscopy. *Advances in Applied Microbiology*, **2010**, 70, 153-86	4.9	141
409	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, 6145-50	5.7	139
408	A metabolome pipeline: from concept to data to knowledge. *Metabolomics*, **2005**, 1, 39-51	4.7	138
407	UbiX is a flavin prenyltransferase required for bacterial ubiquinone biosynthesis. *Nature*, **2015**, 522, 502-6	50.4	136
406	Genetic algorithm optimization for pre-processing and variable selection of spectroscopic data. *Bioinformatics*, **2005**, 21, 860-8	7.2	132
405	1H NMR, GC-EI-TOFMS, and data set correlation for fruit metabolomics: application to spatial metabolite analysis in melon. *Analytical Chemistry*, **2009**, 81, 2884-94	7.8	131
404	Illuminating disease and enlightening biomedicine: Raman spectroscopy as a diagnostic tool. *Analyst, The*, **2013**, 138, 3871-84	5	130
403	Effective quenching processes for physiologically valid metabolite profiling of suspension cultured Mammalian cells. *Analytical Chemistry*, **2009**, 81, 174-83	7.8	125
402	SERS Detection of Multiple Antimicrobial-Resistant Pathogens Using Nanosensors. *Analytical Chemistry*, **2017**, 89, 12666-12673	7.8	122
401	Metabolomics and systems pharmacology: why and how to model the human metabolic network for drug discovery. *Drug Discovery Today*, **2014**, 19, 171-82	8.8	122

400	Chemometric discrimination of unfractionated plant extracts analyzed by electrospray mass spectrometry. *Phytochemistry*, **2003**, 62, 859-63	4	121
399	Systems biology guided by XCMS Online metabolomics. *Nature Methods*, **2017**, 14, 461-462	21.6	120
398	Characterization of microorganisms using UV resonance Raman spectroscopy and chemometrics. *Analytical Chemistry*, **2004**, 76, 585-91	7.8	118
397	Exhaled breath analysis: a review of 'breath-taking' methods for off-line analysis. *Metabolomics*, **2017**, 13, 110	4.7	117
396	Metabolomic analysis of the interaction between plants and herbivores. *Metabolomics*, **2009**, 5, 150-161	4.7	117
395	Portable, quantitative detection of Bacillus bacterial spores using surface-enhanced Raman scattering. *Analytical Chemistry*, **2013**, 85, 3297-302	7.8	116
394	Metabolic profiling using direct infusion electrospray ionisation mass spectrometry for the characterisation of olive oils. *Analyst, The*, **2002**, 127, 1457-62	5	116
393	Influence of missing values substitutes on multivariate analysis of metabolomics data. *Metabolites*, **2014**, 4, 433-52	5.6	115
392	Clinical applications of infrared and Raman spectroscopy: state of play and future challenges. *Analyst, The*, **2018**, 143, 1735-1757	5	114
391	Simultaneous detection and quantification of three bacterial meningitis pathogens by SERS. *Chemical Science*, **2014**, 5, 1030-1040	9.4	114
390	Metabolomic approaches reveal that phosphatidic and phosphatidyl glycerol phospholipids are major discriminatory non-polar metabolites in responses by Brachypodium distachyon to challenge by Magnaporthe grisea. *Plant Journal*, **2006**, 46, 351-68	6.9	110
389	COordination of Standards in MetabOlomicS (COSMOS): facilitating integrated metabolomics data access. *Metabolomics*, **2015**, 11, 1587-1597	4.7	109
388	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	3.8	109
387	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	4.7	109
386	Multiplexed detection of six labelled oligonucleotides using surface enhanced resonance Raman scattering (SERRS). *Analyst, The*, **2008**, 133, 1505-12	5	108
385	Ultrasensitive Colorimetric Detection of Murine Norovirus Using NanoZyme Aptasensor. *Analytical Chemistry*, **2019**, 91, 3270-3276	7.8	108
384	Inter-laboratory reproducibility of fast gas chromatography-electron impact-time of flight mass spectrometry (GC-EI-TOF/MS) based plant metabolomics. *Metabolomics*, **2009**, 5, 479-496	4.7	107
383	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, 6689-97	7.8	106

382	Non-invasive metabolomic analysis of breath using differential mobility spectrometry in patients with chronic obstructive pulmonary disease and healthy smokers. *Analyst, The*, **2010**, 135, 315-20	5	106
381	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	6.6	105
380	Flow infusion electrospray ionisation mass spectrometry for high throughput, non-targeted metabolite fingerprinting: a review. *Metabolomics*, **2013**, 9, 4-29	4.7	104
379	Functional genomics via metabolic footprinting: monitoring metabolite secretion by Escherichia coli tryptophan metabolism mutants using FT-IR and direct injection electrospray mass spectrometry. *Comparative and Functional Genomics*, **2003**, 4, 376-91		104
378	Surface-enhanced Raman scattering from intracellular and extracellular bacterial locations. *Analytical Chemistry*, **2008**, 80, 6741-6	7.8	102
377	Extensive metabolic cross-talk in melon fruit revealed by spatial and developmental combinatorial metabolomics. *New Phytologist*, **2011**, 190, 683-96	9.8	101
376	Pyrolysis mass spectrometry and its applications in biotechnology. *Current Opinion in Biotechnology*, **1996**, 7, 20-8	11.4	100
375	Taking your breath away: metabolomics breathes life in to personalized medicine. *Trends in Biotechnology*, **2014**, 32, 538-48	15.1	98
374	An automated Design-Build-Test-Learn pipeline for enhanced microbial production of fine chemicals. *Communications Biology*, **2018**, 1, 66	6.7	97
373	Variable selection in discriminant partial least-squares analysis. *Analytical Chemistry*, **1998**, 70, 4126-33	7.8	97
372	Metabolic footprinting as a tool for discriminating between brewing yeasts. *Yeast*, **2007**, 24, 667-79	3.4	96
371	Untargeted metabolic profiling identifies altered serum metabolites of type 2 diabetes mellitus in a prospective, nested case control study. *Clinical Chemistry*, **2015**, 61, 487-97	5.5	94
370	Rapid identification of closely related muscle foods by vibrational spectroscopy and machine learning. *Analyst, The*, **2005**, 130, 1648-54	5	94
369	Metabolite profiling of recombinant CHO cells: designing tailored feeding regimes that enhance recombinant antibody production. *Biotechnology and Bioengineering*, **2011**, 108, 3025-31	4.9	92
368	A comparison of Raman and FT-IR spectroscopy for the prediction of meat spoilage. *Food Control*, **2013**, 29, 461-470	6.2	90
367	Fourier transform infrared spectroscopy and multivariate analysis for the detection and quantification of different milk species. *Journal of Dairy Science*, **2010**, 93, 5651-60	4	88
366	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	7.8	87
365	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, 118-28	3.5	86

364	Data standards can boost metabolomics research, and if there is a will, there is a way. *Metabolomics*, **2016**, 12, 14	4.7	85
363	Recent developments in quantitative SERS: Moving towards absolute quantification. *TrAC - Trends in Analytical Chemistry*, **2018**, 102, 359-368	14.6	84
362	Discrimination of aerobic endospore-forming bacteria via electrospray-lonization mass spectrometry of whole cell suspensions. *Analytical Chemistry*, **2001**, 73, 4134-44	7.8	84
361	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	4.7	82
360	Rapid identification using pyrolysis mass spectrometry and artificial neural networks of Propionibacterium acnes isolated from dogs. *Journal of Applied Bacteriology*, **1994**, 76, 124-34		82
359	A comparative investigation of modern feature selection and classification approaches for the analysis of mass spectrometry data. *Analytica Chimica Acta*, **2014**, 829, 1-8	6.6	81
358	Rapid and quantitative detection of the microbial spoilage in milk using Fourier transform infrared spectroscopy and chemometrics. *Analyst, The*, **2008**, 133, 1424-31	5	81
357	Ultra-violet resonance Raman spectroscopy for the rapid discrimination of urinary tract infection bacteria. *FEMS Microbiology Letters*, **2004**, 232, 127-32	2.9	81
356	Electronic cigarette exposure triggers neutrophil inflammatory responses. *Respiratory Research*, **2016**, 17, 56	7.3	80
355	Raman activated cell ejection for isolation of single cells. *Analytical Chemistry*, **2013**, 85, 10697-701	7.8	80
354	Progress toward the Rapid Nondestructive Assessment of the Floral Origin of European Honey Using Dispersive Raman Spectroscopy. *Applied Spectroscopy*, **2002**, 56, 521-527	3.1	80
353	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	6.6	75
352	Accumulation of ionic liquids in Escherichia colicells. *Green Chemistry*, **2008**, 10, 836	10	74
351	Monitoring the mode of action of antibiotics using Raman spectroscopy: investigating subinhibitory effects of amikacin on Pseudomonas aeruginosa. *Analytical Chemistry*, **2005**, 77, 2901-6	7.8	74
350	Monitoring of complex industrial bioprocesses for metabolite concentrations using modern spectroscopies and machine learning: application to gibberellic acid production. *Biotechnology and Bioengineering*, **2002**, 78, 527-38	4.9	74
349	Neural networks and olive oil. *Nature*, **1992**, 359, 594-594	50.4	73
348	Explanatory analysis of spectroscopic data using machine learning of simple, interpretable rules. *Vibrational Spectroscopy*, **2003**, 32, 33-45	2.1	72
347	Dual metabolomics: a novel approach to understanding plant-pathogen interactions. *Phytochemistry*, **2010**, 71, 590-7	4	71

346	Metabolomics for the masses: The future of metabolomics in a personalized world. *European Journal of Molecular and Clinical Medicine*, **2017**, 3, 294-305	0.7	70
345	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	3.1	70
344	Meat, the metabolites: an integrated metabolite profiling and lipidomics approach for the detection of the adulteration of beef with pork. *Analyst, The*, **2016**, 141, 2155-64	5	69
343	Metabolomic approaches reveal that cell wall modifications play a major role in ethylene-mediated resistance against Botrytis cinerea. *Plant Journal*, **2011**, 67, 852-68	6.9	69
342	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	4.4	69
341	Rapid monitoring of antibiotics using Raman and surface enhanced Raman spectroscopy. *Analyst, The*, **2005**, 130, 1019-26	5	68
340	Absolute Quantification of Uric Acid in Human Urine Using Surface Enhanced Raman Scattering with the Standard Addition Method. *Analytical Chemistry*, **2017**, 89, 2472-2477	7.8	67
339	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	6.6	65
338	Plant metabolomics and its potential for systems biology research background concepts, technology, and methodology. *Methods in Enzymology*, **2011**, 500, 299-336	1.7	63
337	Screening ionic liquids for use in biotransformations with whole microbial cells. *Green Chemistry*, **2011**, 13, 1843	10	63
336	MALDI-MS and multivariate analysis for the detection and quantification of different milk species. *Analytical and Bioanalytical Chemistry*, **2011**, 399, 3491-502	4.4	63
335	PYCHEM: a multivariate analysis package for python. *Bioinformatics*, **2006**, 22, 2565-6	7.2	63
334	Correction of mass spectral drift using artificial neural networks. *Analytical Chemistry*, **1996**, 68, 271-80	7.8	63
333	Using a biphasic ionic liquid/water reaction system to improve oxygenase-catalysed biotransformation with whole cells. *Green Chemistry*, **2008**, 10, 685	10	62
332	Investigating plant-plant interference by metabolic fingerprinting. *Phytochemistry*, **2003**, 63, 705-10	4	62
331	Metabolic acclimation to hypoxia revealed by metabolite gradients in melon fruit. *Journal of Plant Physiology*, **2010**, 167, 242-5	3.6	61
330	Matrix-suppressed laser desorption/ionisation mass spectrometry and its suitability for metabolome analyses. *Rapid Communications in Mass Spectrometry*, **2006**, 20, 1192-8	2.2	61
329	Making sense of the metabolome using evolutionary computation: seeing the wood with the trees. *Journal of Experimental Botany*, **2005**, 56, 245-54	7	60

328	Rapid identification of species within the Mycobacterium tuberculosis complex by artificial neural network analysis of pyrolysis mass spectra. *Journal of Medical Microbiology*, **1994**, 40, 170-3	3.2	60
327	Combining Raman and FT-IR spectroscopy with quantitative isotopic labeling for differentiation of E. coli cells at community and single cell levels. *Analytical Chemistry*, **2015**, 87, 4578-86	7.8	59
326	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, 5681-7	7.8	59
325	Rapid and quantitative analysis and bioprocesses using pyrolysis mass spectrometry and neural networks: application to indole production. *Analytica Chimica Acta*, **1993**, 279, 17-26	6.6	59
324	Novel noninvasive identification of biomarkers by analytical profiling of chronic wounds using volatile organic compounds. *Wound Repair and Regeneration*, **2010**, 18, 391-400	3.6	58
323	Metabolic responses of eukaryotic microalgae to environmental stress limit the ability of FT-IR spectroscopy for species identification. *Algal Research*, **2015**, 11, 148-155	5	57
322	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, 923-31	7.8	57
321	Exhaled Volatile Organic Compounds of Infection: A Systematic Review. *ACS Infectious Diseases*, **2017**, 3, 695-710	5.5	53
320	Characterisation of intact microorganisms using electrospray ionisation mass spectrometry. *FEMS Microbiology Letters*, **1999**, 176, 17-24	2.9	53
319	Computational tools and workflows in metabolomics: An international survey highlights the opportunity for harmonisation through Galaxy. *Metabolomics*, **2017**, 13, 12	4.7	52
318	Detection and quantification of bacterial spoilage in milk and pork meat using MALDI-TOF-MS and multivariate analysis. *Analytical Chemistry*, **2012**, 84, 5951-8	7.8	52
317	Reverse and Multiple Stable Isotope Probing to Study Bacterial Metabolism and Interactions at the Single Cell Level. *Analytical Chemistry*, **2016**, 88, 9443-9450	7.8	52
316	Metabolomics in melon: a new opportunity for aroma analysis. *Phytochemistry*, **2014**, 99, 61-72	4	51
315	Acclimation of metabolism to light in Arabidopsis thaliana: the glucose 6-phosphate/phosphate translocator GPT2 directs metabolic acclimation. *Plant, Cell and Environment*, **2015**, 38, 1404-17	8.4	51
314	Genetic programming: a novel method for the quantitative analysis of pyrolysis mass spectral data. *Analytical Chemistry*, **1997**, 69, 4381-9	7.8	51
313	Subsurface biomolecular imaging of Streptomyces coelicolor using secondary ion mass spectrometry. *Analytical Chemistry*, **2008**, 80, 1942-51	7.8	51
312	Metabolic fingerprints of Mycobacterium bovis cluster with molecular type: implications for genotype-phenotype links. *Microbiology (United Kingdom)*, **2006**, 152, 2757-2765	2.9	51
311	A comparison of different chemometrics approaches for the robust classification of electronic nose data. *Analytical and Bioanalytical Chemistry*, **2014**, 406, 7581-90	4.4	50

310	Metabolomics-assisted synthetic biology. *Current Opinion in Biotechnology*, **2012**, 23, 22-8	11.4	50
309	Integration of metabolomics in heart disease and diabetes research: current achievements and future outlook. *Bioanalysis*, **2011**, 3, 2205-22	2.1	50
308	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, 1276-86	2.2	50
307	A novel untargeted metabolomics correlation-based network analysis incorporating human metabolic reconstructions. *BMC Systems Biology*, **2013**, 7, 107	3.5	49
306	Comparison of diffuse-reflectance absorbance and attenuated total reflectance FT-IR for the discrimination of bacteria. *Analyst, The*, **2004**, 129, 1118-22	5	49
305	The influence of scaling metabolomics data on model classification accuracy. *Metabolomics*, **2015**, 11, 684-695	4.7	48
304	On mass spectrometer instrument standardization and interlaboratory calibration transfer using neural networks. *Analytica Chimica Acta*, **1997**, 348, 511-532	6.6	48
303	A flavour of omics approaches for the detection of food fraud. *Current Opinion in Food Science*, **2016**, 10, 7-15	9.8	47
302	Detection of small genotypic changes in Escherichia coli by pyrolysis mass spectroscopy. *FEMS Microbiology Letters*, **1990**, 71, 133-137	2.9	47
301	Raman spectroscopy: lighting up the future of microbial identification. *Future Microbiology*, **2011**, 6, 991-7	2.9	46
300	Contribution of pyrolysis-mass spectrometry (Py-MS) to authenticity testing of honey. *Journal of Analytical and Applied Pyrolysis*, **2001**, 60, 79-87	6	46
299	Rapid screening for metabolite overproduction in fermentor broths, using pyrolysis mass spectrometry with multivariate calibration and artificial neural networks. *Biotechnology and Bioengineering*, **1994**, 44, 1205-16	4.9	46
298	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	6.6	46
297	Quantitative Online Liquid Chromatography-Surface-Enhanced Raman Scattering (LC-SERS) of Methotrexate and its Major Metabolites. *Analytical Chemistry*, **2017**, 89, 6702-6709	7.8	44
296	Discovery of Volatile Biomarkers of Parkinson's Disease from Sebum. *ACS Central Science*, **2019**, 5, 599-606	10.8	44
295	Predicting human embryo viability: the road to non-invasive analysis of the secretome using metabolic footprinting. *Reproductive BioMedicine Online*, **2007**, 15, 296-302	4	44
294	The rapid identification of Acinetobacter species using Fourier transform infrared spectroscopy. *Journal of Applied Microbiology*, **2004**, 96, 328-39	4.7	44
293	Surface-Enhanced Raman Scattering (SERS) in Microbiology: Illumination and Enhancement of the Microbial World. *Applied Spectroscopy*, **2018**, 72, 987-1000	3.1	43

292	Surveillance for lower airway pathogens in mechanically ventilated patients by metabolomic analysis of exhaled breath: a case-control study. *Thorax*, **2015**, 70, 320-5	7.3	43
291	Structural, spectroscopic and redox properties of uranyl complexes with a maleonitrile containing ligand. *Dalton Transactions*, **2011**, 40, 5939-52	4.3	43
290	Through-container, extremely low concentration detection of multiple chemical markers of counterfeit alcohol using a handheld SORS device. *Scientific Reports*, **2017**, 7, 12082	4.9	42
289	The importance of protonation in the investigation of protein phosphorylation using Raman spectroscopy and Raman optical activity. *Analytical Chemistry*, **2011**, 83, 7978-83	7.8	42
288	Rapid monitoring of recombinant antibody production by mammalian cell cultures using fourier transform infrared spectroscopy and chemometrics. *Biotechnology and Bioengineering*, **2010**, 106, 432-42	4.9	42
287	Monitoring the glycosylation status of proteins using Raman spectroscopy. *Analytical Chemistry*, **2011**, 83, 6074-81	7.8	41
286	Quantitative detection of metabolites using matrix-assisted laser desorption/ionization mass spectrometry with 9-aminoacridine as the matrix. *Rapid Communications in Mass Spectrometry*, **2007** , 21, 2072-8	2.2	41
285	Differentiation of Micromonospora isolates from a coastal sediment in Wales on the basis of Fourier transform infrared spectroscopy, 16S rRNA sequence analysis, and the amplified fragment length polymorphism technique. *Applied and Environmental Microbiology*, **2004**, 70, 6619-27	4.8	41
284	Metabolomics the way forward. *Metabolomics*, **2005**, 1, 1-2	4.7	41
283	Rapid analysis of the expression of heterologous proteins in Escherichia coli using pyrolysis mass spectrometry and Fourier transform infrared spectroscopy with chemometrics: application to alpha 2-interferon production. *Journal of Biotechnology*, **1999**, 72, 157-67	3.7	41
282	Identification and discrimination of oral asaccharolytic Eubacterium spp. by pyrolysis mass spectrometry and artificial neural networks. *Current Microbiology*, **1996**, 32, 77-84	2.4	41
281	Explanatory Analysis of the Metabolome Using Genetic Programming of Simple, Interpretable Rules. *Genetic Programming and Evolvable Machines*, **2000**, 1, 243-258	2	40
280	Impact of silver(I) on the metabolism of Shewanella oneidensis. *Journal of Bacteriology*, **2010**, 192, 1143-50	3.9	39
279	VOC-based metabolic profiling for food spoilage detection with the application to detecting Salmonella typhimurium-contaminated pork. *Analytical and Bioanalytical Chemistry*, **2010**, 397, 2439-49	4.4	39
278	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, 516-39		39
277	Differentiation of brewing yeast strains by pyrolysis mass spectrometry and Fourier transform infrared spectroscopy. *Yeast*, **1998**, 14, 885-93	3.4	38
276	Relatedness of medically important strains of Saccharomyces cerevisiae as revealed by phylogenetics and metabolomics. *Yeast*, **2008**, 25, 501-12	3.4	38
275	Characterization of exopolymers of aquatic bacteria by pyrolysis-mass spectrometry. *Applied and Environmental Microbiology*, **1991**, 57, 1595-601	4.8	38

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