

Roy Goodacre

List of Publications by Year in Descending Order

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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.

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	Reference materials for MS-based untargeted metabolomics and lipidomics: a review by the metabolomics quality assurance and quality control consortium (mQACC).. <i>Metabolomics</i> , 2022 , 18, 24	4.7	4
452	Simultaneous Raman and Infrared Spectroscopy of Stable Isotope Labelled Escherichia coli. <i>Sensors</i> , 2022 , 22, 3928	3.8	1
451	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
450	Breath and plasma metabolomics to assess inflammation in acute stroke. <i>Scientific Reports</i> , 2021 , 11, 21949	4.9	1
449	Metabolomics of sebum reveals lipid dysregulation in Parkinson's disease. <i>Nature Communications</i> , 2021 , 12, 1592	17.4	27
448	Untargeted Molecular Analysis of Exhaled Breath as a Diagnostic Test for Ventilator-Associated Lower Respiratory Tract Infections (BreathDx). <i>Thorax</i> , 2021 ,	7.3	1
447	The Role of Raman Spectroscopy Within Quantitative Metabolomics. <i>Annual Review of Analytical Chemistry</i> , 2021 , 14, 323-345	12.5	5
446	Assessment of Transdermal Delivery of Topical Compounds in Skin Scarring Using a Novel Combined Approach of Raman Spectroscopy and High-Performance Liquid Chromatography. <i>Advances in Wound Care</i> , 2021 , 10, 1-12	4.8	0
445	Discrimination of bacteria using whole organism fingerprinting: the utility of modern physicochemical techniques for bacterial typing. <i>Analyst, The</i> , 2021 , 146, 770-788	5	12
444	Detection and quantification of exhaled volatile organic compounds in mechanically ventilated patients - comparison of two sampling methods. <i>Analyst, The</i> , 2021 , 146, 222-231	5	2
443	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
442	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
441	Rapid Spectroscopic Liquid Biopsy for the Universal Detection of Brain Tumours. <i>Cancers</i> , 2021 , 13,	6.6	7
440	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
439	Portable through Bottle SORS for the Authentication of Extra Virgin Olive Oil. <i>Applied Sciences (Switzerland)</i> , 2021 , 11, 8347	2.6	4
438	Comparing root exudate collection techniques: An improved hybrid method. <i>Soil Biology and Biochemistry</i> , 2021 , 161, 108391	7.5	6
437	Spectral artefacts induced by moving targets in live hyperspectral stimulated Raman spectroscopy: The case of lipid droplets in yeast cells. <i>Clinical Spectroscopy</i> , 2021 , 3, 100014	16	0

436	Effects of high relative humidity and dry purging on VOCs obtained during breath sampling on common sorbent tubes. <i>Journal of Breath Research</i> , 2020 , 14, 046006	3.1	6
435	Raman Spectroscopy to Monitor Post-Translational Modifications and Degradation in Monoclonal Antibody Therapeutics. <i>Analytical Chemistry</i> , 2020 , 92, 10381-10389	7.8	13
434	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
433	Surface Enhanced Raman Spectroscopy for Quantitative Analysis: Results of a Large-Scale European Multi-Instrument Interlaboratory Study. <i>Analytical Chemistry</i> , 2020 , 92, 4053-4064	7.8	25
432	Radiation Tolerance of , a Cyanobacterium Relevant to the First Generation Magnox Storage Pond. <i>Frontiers in Microbiology</i> , 2020 , 11, 515	5.7	6
431	Quantification of protein glycation using vibrational spectroscopy. <i>Analyst, The</i> , 2020 , 145, 3686-3696	5	5
430	The role of metabolomics in personalized medicine 2020 , 227-244		
429	Development of a sensor device with polymer-coated piezoelectric micro-cantilevers for detection of volatile organic compounds. <i>Measurement Science and Technology</i> , 2020 , 31, 035103	2	3
428	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
427	Rapid differentiation of <i>Campylobacter jejuni</i> cell wall mutants using Raman spectroscopy, SERS and mass spectrometry combined with chemometrics. <i>Analyst, The</i> , 2020 , 145, 1236-1249	5	11
426	Evaluation of Sample Preparation Methods for Inter-Laboratory Metabolomics Investigation of TK24. <i>Metabolites</i> , 2020 , 10,	5.6	1
425	Targeting Methionine Synthase in a Fungal Pathogen Causes a Metabolic Imbalance That Impacts Cell Energetics, Growth, and Virulence. <i>MBio</i> , 2020 , 11,	7.8	4
424	Comparability of Raman Spectroscopic Configurations: A Large Scale Cross-Laboratory Study. <i>Analytical Chemistry</i> , 2020 , 92, 15745-15756	7.8	22
423	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
422	Sensitive and selective detection of DNA fragments associated with <i>Ganoderma boninense</i> by DNA-nanoparticle conjugate hybridisation. <i>Journal of Materials Science</i> , 2020 , 55, 14965-14979	4.3	1
421	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
420	Present and Future of Surface-Enhanced Raman Scattering. <i>ACS Nano</i> , 2020 , 14, 28-117	16.7	1000
419	Comparative Metabolomics and Molecular Phylogenetics of Melon (, Cucurbitaceae) Biodiversity. <i>Metabolites</i> , 2020 , 10,	5.6	19

418	Detection of the adulteration of fresh coconut water via NMR spectroscopy and chemometrics. <i>Analyst, The</i> , 2019 , 144, 1401-1408	5	11
417	Central Metabolism Is Tuned to the Availability of Oxygen in Developing Melon Fruit. <i>Frontiers in Plant Science</i> , 2019 , 10, 594	6.2	5
416	The blind men and the elephant: challenges in the analysis of complex natural mixtures. <i>Faraday Discussions</i> , 2019 , 218, 524-539	3.6	3
415	Circadian rhythm of exhaled biomarkers in health and asthma. <i>European Respiratory Journal</i> , 2019 , 54,	13.6	24
414	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
413	Polymer Pen Lithography-Fabricated DNA Arrays for Highly Sensitive and Selective Detection of Unamplified DNA. <i>Polymers</i> , 2019 , 11,	4.5	8
412	Discovery of Volatile Biomarkers of Parkinson's Disease from Sebum. <i>ACS Central Science</i> , 2019 , 5, 599-606	6.8	44
411	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
410	Enhancing Disease Diagnosis: Biomedical Applications of Surface-Enhanced Raman Scattering. <i>Applied Sciences (Switzerland)</i> , 2019 , 9, 1163	2.6	32
409	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
408	Rapid quantification of the adulteration of fresh coconut water by dilution and sugars using Raman spectroscopy and chemometrics. <i>Food Chemistry</i> , 2019 , 272, 157-164	8.5	26
407	Omic Methods For the Detection of Foodborne Pathogens 2019 , 364-370		3
406	Dealing with complexity: general discussion. <i>Faraday Discussions</i> , 2019 , 218, 138-156	3.6	1
405	High resolution techniques: general discussion. <i>Faraday Discussions</i> , 2019 , 218, 247-267	3.6	3
404	Data mining and visualisation: general discussion. <i>Faraday Discussions</i> , 2019 , 218, 354-371	3.6	2
403	Metabolic dysregulation in vitamin E and carnitine shuttle energy mechanisms associate with human frailty. <i>Nature Communications</i> , 2019 , 10, 5027	17.4	35
402	Exhaled breath metabolomics reveals a pathogen-specific response in a rat pneumonia model for two human pathogenic bacteria: a proof-of-concept study. <i>American Journal of Physiology - Lung Cellular and Molecular Physiology</i> , 2019 , 316, L751-L756	5.8	5
401	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

400	Biochemical signatures of acclimation by <i>Chlamydomonas reinhardtii</i> to different ionic stresses. <i>Algal Research</i> , 2019 , 37, 83-91	5	6
399	Ultrasensitive Colorimetric Detection of Murine Norovirus Using NanoZyme Aptasensor. <i>Analytical Chemistry</i> , 2019 , 91, 3270-3276	7.8	108
398	Rapid through-container detection of fake spirits and methanol quantification with handheld Raman spectroscopy. <i>Analyst, The</i> , 2018 , 144, 324-330	5	31
397	Clinical applications of infrared and Raman spectroscopy: state of play and future challenges. <i>Analyst, The</i> , 2018 , 143, 1735-1757	5	114
396	Improved Descriptors for the Quantitative Structure-Activity Relationship Modeling of Peptides and Proteins. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 234-243	6.1	22
395	Surface-Enhanced Raman Scattering (SERS) in Microbiology: Illumination and Enhancement of the Microbial World. <i>Applied Spectroscopy</i> , 2018 , 72, 987-1000	3.1	43
394	Recent developments in quantitative SERS: Moving towards absolute quantification. <i>TrAC - Trends in Analytical Chemistry</i> , 2018 , 102, 359-368	14.6	84
393	Headspace volatile organic compounds from bacteria implicated in ventilator-associated pneumonia analysed by TD-GC/MS. <i>Journal of Breath Research</i> , 2018 , 12, 026002	3.1	19
392	A Novel Adaptation Mechanism Underpinning Algal Colonization of a Nuclear Fuel Storage Pond. <i>MBio</i> , 2018 , 9,	7.8	15
391	Development of an adaptable headspace sampling method for metabolic profiling of the fungal volatome. <i>Analyst, The</i> , 2018 , 143, 4155-4162	5	10
390	pH plays a role in the mode of action of trimethoprim on <i>Escherichia coli</i> . <i>PLoS ONE</i> , 2018 , 13, e0200272	3.7	9
389	TD/GC-MS analysis of volatile markers emitted from mono- and co-cultures of and in artificial sputum. <i>Metabolomics</i> , 2018 , 14, 66	4.7	17
388	Volatile organic compound signature from co-culture of lung epithelial cell line with <i>Pseudomonas aeruginosa</i> . <i>Analyst, The</i> , 2018 , 143, 3148-3155	5	17
387	An automated Design-Build-Test-Learn pipeline for enhanced microbial production of fine chemicals. <i>Communications Biology</i> , 2018 , 1, 66	6.7	97
386	Progress in Chemometrics and Biostatistics for Plant Applications, or: A Good Red Wine is a Bad White Wine 2018 , 317-342		
385	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
384	Elevated luteinizing hormone despite normal testosterone levels in older men-natural history, risk factors and clinical features. <i>Clinical Endocrinology</i> , 2018 , 88, 479-490	3.4	18
383	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

382	Mitochondrial aconitase is a key regulator of energy production for growth and protein expression in Chinese hamster ovary cells. <i>Metabolomics</i> , 2018 , 14, 136	4.7	9
381	Translation Stress Positively Regulates MscL-Dependent Excretion of Cytoplasmic Proteins. <i>MBio</i> , 2018 , 9,	7.8	14
380	Guidelines and considerations for the use of system suitability and quality control samples in mass spectrometry assays applied in untargeted clinical metabolomic studies. <i>Metabolomics</i> , 2018 , 14, 72	4.7	303
379	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
378	Computational tools and workflows in metabolomics: An international survey highlights the opportunity for harmonisation through Galaxy. <i>Metabolomics</i> , 2017 , 13, 12	4.7	52
377	Detection of glycosylation and iron-binding protein modifications using Raman spectroscopy. <i>Analyst, The</i> , 2017 , 142, 808-814	5	11
376	Ethnic differences in male reproductive hormones and relationships with adiposity and insulin resistance in older men. <i>Clinical Endocrinology</i> , 2017 , 86, 660-668	3.4	5
375	Quantitative detection of codeine in human plasma using surface-enhanced Raman scattering via adaptation of the isotopic labelling principle. <i>Analyst, The</i> , 2017 , 142, 1099-1105	5	23
374	Systems biology guided by XCMS Online metabolomics. <i>Nature Methods</i> , 2017 , 14, 461-462	21.6	120
373	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
372	Two Glycerol-3-Phosphate Dehydrogenases from Have Distinct Roles in Lipid Metabolism. <i>Plant Physiology</i> , 2017 , 174, 2083-2097	6.6	26
371	Metabolomics for the masses: The future of metabolomics in a personalized world. <i>European Journal of Molecular and Clinical Medicine</i> , 2017 , 3, 294-305	0.7	70
370	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
369	Quantitative detection of isotopically enriched E. coli cells by SERS. <i>Faraday Discussions</i> , 2017 , 205, 331-343	3.4	19
368	Recommendations on the Implementation of Genetic Algorithms for the Directed Evolution of Enzymes for Industrial Purposes. <i>ChemBioChem</i> , 2017 , 18, 1087-1097	3.8	8
367	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
366	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
365	SERS Detection of Multiple Antimicrobial-Resistant Pathogens Using Nanosensors. <i>Analytical Chemistry</i> , 2017 , 89, 12666-12673	7.8	122

364	Exhaled breath analysis: a review of 'breath-taking' methods for off-line analysis. <i>Metabolomics</i> , 2017 , 13, 110	4.7	117
363	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
362	Exhaled Volatile Organic Compounds of Infection: A Systematic Review. <i>ACS Infectious Diseases</i> , 2017 , 3, 695-710	5.5	53
361	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
360	Ultrasensitive and towards single molecule SERS: general discussion. <i>Faraday Discussions</i> , 2017 , 205, 291-330	3.6	9
359	SERS in biology/biomedical SERS: general discussion. <i>Faraday Discussions</i> , 2017 , 205, 429-456	3.6	15
358	Analytical SERS: general discussion. <i>Faraday Discussions</i> , 2017 , 205, 561-600	3.6	9
357	Theory of SERS enhancement: general discussion. <i>Faraday Discussions</i> , 2017 , 205, 173-211	3.6	21
356	Towards improved quantitative analysis using surface-enhanced Raman scattering incorporating internal isotope labelling. <i>Analytical Methods</i> , 2017 , 9, 6636-6644	3.2	15
355	Increased intracellular proteolysis reduces disease severity in an ER stress-associated dwarfism. <i>Journal of Clinical Investigation</i> , 2017 , 127, 3861-3865	15.9	38
354	FUM2, a Cytosolic Fumarase, Is Essential for Acclimation to Low Temperature in <i>Arabidopsis thaliana</i> . <i>Plant Physiology</i> , 2016 , 172, 118-27	6.6	32
353	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
352	A flavour of omics approaches for the detection of food fraud. <i>Current Opinion in Food Science</i> , 2016 , 10, 7-15	9.8	47
351	SERS of meso-droplets supported on superhydrophobic wires allows exquisitely sensitive detection of dipicolinic acid, an anthrax biomarker, considerably below the infective dose. <i>Chemical Communications</i> , 2016 , 52, 9925-8	5.8	31
350	Rapid discrimination of <i>Enterococcus faecium</i> strains using phenotypic analytical techniques. <i>Analytical Methods</i> , 2016 , 8, 7603-7613	3.2	6
349	Intermittent energy restriction induces changes in breast gene expression and systemic metabolism. <i>Breast Cancer Research</i> , 2016 , 18, 57	8.3	22
348	Biofluids and other techniques: general discussion. <i>Faraday Discussions</i> , 2016 , 187, 575-601	3.6	10
347	Spectral Pathology: general discussion. <i>Faraday Discussions</i> , 2016 , 187, 155-86	3.6	4

346	Single cell analysis/data handling: general discussion. <i>Faraday Discussions</i> , 2016 , 187, 299-327	3.6	4
345	Clinical Spectroscopy: general discussion. <i>Faraday Discussions</i> , 2016 , 187, 429-60	3.6	6
344	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
343	Electronic cigarette exposure triggers neutrophil inflammatory responses. <i>Respiratory Research</i> , 2016 , 17, 56	7.3	80
342	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
341	Data standards can boost metabolomics research, and if there is a will, there is a way. <i>Metabolomics</i> , 2016 , 12, 14	4.7	85
340	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
339	Metabolomics reveals the physiological response of <i>Pseudomonas putida</i> KT2440 (UWC1) after pharmaceutical exposure. <i>Molecular BioSystems</i> , 2016 , 12, 1367-77		5
338	Meat, the metabolites: an integrated metabolite profiling and lipidomics approach for the detection of the adulteration of beef with pork. <i>Analyst, The</i> , 2016 , 141, 2155-64	5	69
337	Detection of Protein Glycosylation Using Tip-Enhanced Raman Scattering. <i>Analytical Chemistry</i> , 2016 , 88, 2105-12	7.8	34
336	High-throughput metabolic screening of microalgae genetic variation in response to nutrient limitation. <i>Metabolomics</i> , 2016 , 12, 9	4.7	28
335	Metabolomic analysis of riboswitch containing <i>E. coli</i> recombinant expression system. <i>Molecular BioSystems</i> , 2016 , 12, 350-61		8
334	Chicken, beams, and <i>Campylobacter</i> : rapid differentiation of foodborne bacteria via vibrational spectroscopy and MALDI-mass spectrometry. <i>Analyst, The</i> , 2016 , 141, 111-22	5	31
333	Towards Improving Point-of-Care Diagnosis of Non-malaria Febrile Illness: A Metabolomics Approach. <i>PLoS Neglected Tropical Diseases</i> , 2016 , 10, e0004480	4.8	11
332	Biochemical Analyses of Sorghum Varieties Reveal Differential Responses to Drought. <i>PLoS ONE</i> , 2016 , 11, e0154423	3.7	36
331	Metabolomics Analysis Reveals the Participation of Efflux Pumps and Ornithine in the Response of <i>Pseudomonas putida</i> DOT-T1E Cells to Challenge with Propranolol. <i>PLoS ONE</i> , 2016 , 11, e0156509	3.7	8
330	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
329	Fractional Factorial Design of MALDI-TOF-MS Sample Preparations for the Optimized Detection of Phospholipids and Acylglycerols. <i>Analytical Chemistry</i> , 2016 , 88, 6301-8	7.8	8

328	Label-Free Surface Enhanced Raman Scattering Approach for High-Throughput Screening of Biocatalysts. <i>Analytical Chemistry</i> , 2016 , 88, 5898-903	7.8	24
327	Reverse and Multiple Stable Isotope Probing to Study Bacterial Metabolism and Interactions at the Single Cell Level. <i>Analytical Chemistry</i> , 2016 , 88, 9443-9450	7.8	52
326	Classification of Bacillus and Brevibacillus species using rapid analysis of lipids by mass spectrometry. <i>Analytical and Bioanalytical Chemistry</i> , 2016 , 408, 7865-7878	4.4	14
325	SYNBIOCHEM-a SynBio foundry for the biosynthesis and sustainable production of fine and speciality chemicals. <i>Biochemical Society Transactions</i> , 2016 , 44, 675-7	5.1	5
324	The androgen receptor gene CAG repeat ?in relation to 4-year changes in ?androgen-sensitive endpoints in ?community-dwelling older European men. <i>European Journal of Endocrinology</i> , 2016 , 175, 583-593	6.5	9
323	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
322	Achieving optimal SERS through enhanced experimental design. <i>Journal of Raman Spectroscopy</i> , 2016 , 47, 59-66	2.3	36
321	Functional Exchangeability of Oxidase and Dehydrogenase Reactions in the Biosynthesis of Hydroxyphenylglycine, a Nonribosomal Peptide Building Block. <i>ACS Synthetic Biology</i> , 2015 , 4, 796-807	5.7	5
320	UbiX is a flavin prenyltransferase required for bacterial ubiquinone biosynthesis. <i>Nature</i> , 2015 , 522, 502-504	6.4	136
319	New cofactor supports β -unsaturated acid decarboxylation via 1,3-dipolar cycloaddition. <i>Nature</i> , 2015 , 522, 497-501	50.4	156
318	Metabolic responses of eukaryotic microalgae to environmental stress limit the ability of FT-IR spectroscopy for species identification. <i>Algal Research</i> , 2015 , 11, 148-155	5	57
317	Detection and quantification of the opioid tramadol in urine using surface enhanced Raman scattering. <i>Analyst, The</i> , 2015 , 140, 5965-70	5	23
316	Profiling of spatial metabolite distributions in wheat leaves under normal and nitrate limiting conditions. <i>Phytochemistry</i> , 2015 , 115, 99-111	4	18
315	Oxidized phosphatidylcholines suggest oxidative stress in patients with medium-chain acyl-CoA dehydrogenase deficiency. <i>Talanta</i> , 2015 , 139, 62-6	6.2	29
314	Molecular phenotyping of a UK population: defining the human serum metabolome. <i>Metabolomics</i> , 2015 , 11, 9-26	4.7	167
313	Application of surface enhanced Raman scattering to the solution based detection of a popular legal high, 5,6-methylenedioxy-2-aminoindane (MDAI). <i>Analyst, The</i> , 2015 , 140, 4399-406	5	20
312	MUSCLE: automated multi-objective evolutionary optimization of targeted LC-MS/MS analysis. <i>Bioinformatics</i> , 2015 , 31, 975-7	7.2	9
311	Combining Raman and FT-IR spectroscopy with quantitative isotopic labeling for differentiation of E. coli cells at community and single cell levels. <i>Analytical Chemistry</i> , 2015 , 87, 4578-86	7.8	59

310	Simultaneous quantification of the boar-taint compounds skatole and androstenone by surface-enhanced Raman scattering (SERS) and multivariate data analysis. <i>Analytical and Bioanalytical Chemistry</i> , 2015 , 407, 7787-95	4.4	10
309	Making colourful sense of Raman images of single cells. <i>Analyt, The</i> , 2015 , 140, 1852-8	5	16
308	Aseptic Raman spectroscopy can detect changes associated with the culture of human dental pulp stromal cells in osteoinductive culture. <i>Analyt, The</i> , 2015 , 140, 7347-54	5	4
307	Point-and-shoot: rapid quantitative detection methods for on-site food fraud analysis [moving out of the laboratory and into the food supply chain. <i>Analytical Methods</i> , 2015 , 7, 9401-9414	3.2	149
306	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
305	Untargeted metabolic profiling identifies altered serum metabolites of type 2 diabetes mellitus in a prospective, nested case control study. <i>Clinical Chemistry</i> , 2015 , 61, 487-97	5.5	94
304	UV resonance Raman spectroscopy: a process analytical tool for host cell DNA and RNA dynamics in mammalian cell lines. <i>Journal of Chemical Technology and Biotechnology</i> , 2015 , 90, 237-243	3.5	14
303	The influence of scaling metabolomics data on model classification accuracy. <i>Metabolomics</i> , 2015 , 11, 684-695	4.7	48
302	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
301	Acclimation of metabolism to light in Arabidopsis thaliana: the glucose 6-phosphate/phosphate translocator GPT2 directs metabolic acclimation. <i>Plant, Cell and Environment</i> , 2015 , 38, 1404-17	8.4	51
300	Detection of early stage changes associated with adipogenesis using Raman spectroscopy under aseptic conditions. <i>Cytometry Part A: the Journal of the International Society for Analytical Cytology</i> , 2015 , 87, 1012-9	4.6	9
299	Metabolic profiling reveals potential metabolic markers associated with Hypoxia Inducible Factor-mediated signalling in hypoxic cancer cells. <i>Scientific Reports</i> , 2015 , 5, 15649	4.9	23
298	PWE-199 Metabolomic profiling in acute pancreatitis; in search of new biomarkers. <i>Gut</i> , 2015 , 64, A299.2-1-300	4.9	300
297	PWE-200 Metabolomic profiling in pancreatic cancer; in search of new biomarkers. <i>Gut</i> , 2015 , 64, A300.1-1-300	4.9	300
296	Metabolomics investigation of recombinant mTNF α production in Streptomyces lividans. <i>Microbial Cell Factories</i> , 2015 , 14, 157	6.4	15
295	Metabolite profiling of CHO cells: Molecular reflections of bioprocessing effectiveness. <i>Biotechnology Journal</i> , 2015 , 10, 1434-45	5.6	33
294	A systematic analysis of TCA Escherichia coli mutants reveals suitable genetic backgrounds for enhanced hydrogen and ethanol production using glycerol as main carbon source. <i>Biotechnology Journal</i> , 2015 , 10, 1750-61	5.6	11
293	Metabolic Profiling of Geobacter sulfurreducens during Industrial Bioprocess Scale-Up. <i>Applied and Environmental Microbiology</i> , 2015 , 81, 3288-98	4.8	21

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4 Fingerprint Spectrometry Methods in Bacillus Systematics 254-270

3 Characterisation of intact microorganisms using electrospray ionisation mass spectrometry 4

2 Untargeted metabolomics of COVID-19 patient serum reveals potential prognostic markers of both severity and outcome 11

1 Root functional traits explain root exudation rate and composition across a range of grassland species. *Journal of Ecology*, 6 10