

David Scott Wishart

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.

410
papers

62,704
citations

100
h-index

248
g-index

429
ext. papers

77,013
ext. citations

8.1
avg, IF

8.29
L-index

#	Paper	IF	Citations
410	Metabolomic Fingerprint of Behavioral Changes in Response to Full-Spectrum Cannabis Extracts.. <i>Frontiers in Pharmacology</i> , 2022 , 13, 831052	5.6	
409	Blood Metabolomic Phenotyping of Dry Cows Could Predict the High Milk Somatic Cells in Early Lactation Preliminary Results. <i>Dairy</i> , 2022 , 3, 59-77	2.6	1
408	Combination of mouse prion protein with detoxified lipopolysaccharide triggers colon genes related to inflammatory, antibacterial, and apoptotic responses.. <i>Research in Veterinary Science</i> , 2022 , 144, 98-107	2.5	
407	Urinary metabolomics to develop predictors for pediatric acute kidney injury.. <i>Pediatric Nephrology</i> , 2022 , 1	3.2	0
406	HMDB 5.0: the Human Metabolome Database for 2022.. <i>Nucleic Acids Research</i> , 2022 , 50, D622-D631	20.1	65
405	Systemic inflammation and metabolic disturbances underlie inpatient mortality among ill children with severe malnutrition.. <i>Science Advances</i> , 2022 , 8, eabj6779	14.3	0
404	Advances in Metabolomics-Driven Diagnostic Breeding and Crop Improvement. <i>Metabolites</i> , 2022 , 12, 511	5.6	1
403	A deep generative model enables automated structure elucidation of novel psychoactive substances. <i>Nature Machine Intelligence</i> , 2021 , 3, 973-984	22.5	4
402	Emerging technologies and their impact on regulatory science. <i>Experimental Biology and Medicine</i> , 2021 , 15353702211052280	3.7	3
401	A Canadian Study of Cisplatin Metabolomics and Nephrotoxicity (ACCENT): A Clinical Research Protocol. <i>Canadian Journal of Kidney Health and Disease</i> , 2021 , 8, 20543581211057708	2.3	0
400	Metabolomics in Exercise and Sports: A Systematic Review. <i>Sports Medicine</i> , 2021 , 1	10.6	2
399	Exploring Biological Impacts of Prenatal Nutrition and Selection for Residual Feed Intake on Beef Cattle Using Omics Technologies: A Review. <i>Frontiers in Genetics</i> , 2021 , 12, 720268	4.5	1
398	CpG-ODN induced antimicrobial immunity in neonatal chicks involves a substantial shift in serum metabolic profiles. <i>Scientific Reports</i> , 2021 , 11, 9028	4.9	0
397	A Comprehensive Targeted Metabolomics Assay for Crop Plant Sample Analysis. <i>Metabolites</i> , 2021 , 11,	5.6	4
396	CyProduct: A Software Tool for Accurately Predicting the Byproducts of Human Cytochrome P450 Metabolism. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 3128-3140	6.1	4
395	Chemical language models enable navigation in sparsely populated chemical space. <i>Nature Machine Intelligence</i> , 2021 , 3, 759-770	22.5	8
394	Targeted metabolomics identifies high performing diagnostic and prognostic biomarkers for COVID-19. <i>Scientific Reports</i> , 2021 , 11, 14732	4.9	11

393	MarkerDB: an online database of molecular biomarkers. <i>Nucleic Acids Research</i> , 2021 , 49, D1259-D1267	20.1	16
392	Predicting PAMPA permeability using the 3D-RISM-KH theory: are we there yet?. <i>Journal of Computer-Aided Molecular Design</i> , 2021 , 35, 261-269	4.2	4
391	Food Constituent and Food Metabolite Databases 2021 , 2-18		2
390	Cloning and high-level expression of monomeric human superoxide dismutase 1 (SOD1) and its interaction with pyrimidine analogs. <i>PLoS ONE</i> , 2021 , 16, e0247684	3.7	0
389	A Cross-Platform Metabolomics Comparison Identifies Serum Metabolite Signatures of Liver Fibrosis Progression in Chronic Hepatitis C Patients. <i>Frontiers in Molecular Biosciences</i> , 2021 , 8, 676349	5.6	2
388	Immunometabolic signatures predict risk of progression to sepsis in COVID-19. <i>PLoS ONE</i> , 2021 , 16, e0256784	2	
387	CFM-ID 4.0: More Accurate ESI-MS/MS Spectral Prediction and Compound Identification. <i>Analytical Chemistry</i> , 2021 , 93, 11692-11700	7.8	11
386	A Targeted Serum Metabolomics GC-MS Approach Identifies Predictive Blood Biomarkers for Retained Placenta in Holstein Dairy Cows. <i>Metabolites</i> , 2021 , 11,	5.6	2
385	A longitudinal dataset of incidence and intervention policy impacts regarding the COVID-19 pandemic in Canadian provinces. <i>Data in Brief</i> , 2021 , 38, 107381	1.2	
384	A Multi-Platform Metabolomics Approach Identifies Urinary Metabolite Signatures That Differentiate Ketotic From Healthy Dairy Cows. <i>Frontiers in Veterinary Science</i> , 2021 , 8, 595983	3.1	4
383	Urinary Metabolomics around Parturition Identifies Metabolite Alterations in Dairy Cows Affected Postpartum by Lameness: Preliminary Study. <i>Dairy</i> , 2020 , 1, 2	2.6	6
382	The Bovine Metabolome. <i>Metabolites</i> , 2020 , 10,	5.6	40
381	Serum metabolomics identifies metabolite panels that differentiate lame dairy cows from healthy ones. <i>Metabolomics</i> , 2020 , 16, 73	4.7	2
380	Effect of Diet on the Vitamin B Profile of Bovine Milk-Based Protein Ingredients. <i>Foods</i> , 2020 , 9,	4.9	3
379	Insights into origins and function of the unexplored majority of the reductive dehalogenase gene family as a result of genome assembly and ortholog group classification. <i>Environmental Sciences: Processes and Impacts</i> , 2020 , 22, 663-678	4.3	13
378	Milk Metabotyping Identifies Metabolite Alterations in the Whole Raw Milk of Dairy Cows with Lameness. <i>Journal of Agricultural and Food Chemistry</i> , 2020 , 68, 4507-4514	5.7	4
377	A High-Performing Plasma Metabolite Panel for Early-Stage Lung Cancer Detection. <i>Cancers</i> , 2020 , 12,	6.6	20
376	Comprehensive Targeted Metabolomic Assay for Urine Analysis. <i>Analytical Chemistry</i> , 2020 , 92, 10627-10634	6.3	15

375	FOBI: an ontology to represent food intake data and associate it with metabolomic data. <i>Database: the Journal of Biological Databases and Curation</i> , 2020 , 2020,	5	18
374	Value-based healthcare delivery through metabolomics-based personalized health platform. <i>Healthcare Management Forum</i> , 2020 , 33, 126-134	1.7	1
373	The Urinary Metabolome of Healthy Newborns. <i>Metabolites</i> , 2020 , 10,	5.6	8
372	Targeted metabolomics highlights perturbed metabolism in the brain of autism spectrum disorder sufferers. <i>Metabolomics</i> , 2020 , 16, 59	4.7	7
371	Perspective: Dietary Biomarkers of Intake and Exposure-Exploration with Omics Approaches. <i>Advances in Nutrition</i> , 2020 , 11, 200-215	10	35
370	Serum metabolic fingerprinting of pre-lameness dairy cows by GC-MS reveals typical profiles that can identify susceptible cows. <i>Journal of Proteomics</i> , 2020 , 213, 103620	3.9	2
369	Mass-spec-based urinary metabotyping around parturition identifies screening biomarkers for subclinical mastitis in dairy cows. <i>Research in Veterinary Science</i> , 2020 , 129, 39-52	2.5	5
368	Gut Microenvironment and Bacterial Invasion in Paediatric Inflammatory Bowel Diseases. <i>Journal of Pediatric Gastroenterology and Nutrition</i> , 2020 , 71, 624-632	2.8	3
367	Workshop report: Toward the development of a human whole stool reference material for metabolomic and metagenomic gut microbiome measurements. <i>Metabolomics</i> , 2020 , 16, 119	4.7	3
366	Serum Metabolite Biomarkers for Predicting Residual Feed Intake (RFI) of Young Angus Bulls. <i>Metabolites</i> , 2020 , 10,	5.6	5
365	Excretory/Secretory Metabolome of the Zoonotic Roundworm Parasite. <i>Biomolecules</i> , 2020 , 10,	5.9	3
364	Metabolomics Profiling of Critically Ill Coronavirus Disease 2019 Patients: Identification of Diagnostic and Prognostic Biomarkers 2020 , 2, e0272		49
363	Candidate serum metabolite biomarkers of residual feed intake and carcass merit in sheep. <i>Journal of Animal Science</i> , 2020 , 98,	0.7	7
362	Exposome-Explorer 2.0: an update incorporating candidate dietary biomarkers and dietary associations with cancer risk. <i>Nucleic Acids Research</i> , 2020 , 48, D908-D912	20.1	15
361	PathBank: a comprehensive pathway database for model organisms. <i>Nucleic Acids Research</i> , 2020 , 48, D470-D478	20.1	35
360	Metabolomic Data Exploration and Analysis with the Human Metabolome Database. <i>Methods in Molecular Biology</i> , 2020 , 2104, 165-184	1.4	5
359	Preparation and characterization of a highly soluble A β peptide variant. <i>Protein Expression and Purification</i> , 2019 , 164, 105480	2	3
358	Comparison of the metabolomic profiles of irritable bowel syndrome patients with ulcerative colitis patients and healthy controls: new insights into pathophysiology and potential biomarkers. <i>Alimentary Pharmacology and Therapeutics</i> , 2019 , 49, 723-732	6.1	20

357	Transformation of polyphenols found in pigmented gluten-free flours during in vitro large intestinal fermentation. <i>Food Chemistry</i> , 2019 , 298, 125068	8.5	20
356	Protocols for NMR Analysis in Livestock Metabolomics. <i>Methods in Molecular Biology</i> , 2019 , 1996, 311-324	4	8
355	A fast, sensitive, single-step colorimetric dipstick assay for quantifying ascorbic acid in urine. <i>Analytical Biochemistry</i> , 2019 , 580, 1-13	3.1	6
354	CFM-ID 3.0: Significantly Improved ESI-MS/MS Prediction and Compound Identification. <i>Metabolites</i> , 2019 , 9,	5.6	126
353	Systems Biology and Multi-Omics Integration: Viewpoints from the Metabolomics Research Community. <i>Metabolites</i> , 2019 , 9,	5.6	236
352	Chemical Composition of Commercial Cow's Milk. <i>Journal of Agricultural and Food Chemistry</i> , 2019 , 67, 4897-4914	5.7	70
351	Porous Nanophotonic Optomechanical Beams for Enhanced Mass Adsorption. <i>ACS Sensors</i> , 2019 , 4, 1197-1203	3	203
350	Non-invasive differentiation of non-rejection kidney injury from acute rejection in pediatric renal transplant recipients. <i>Pediatric Transplantation</i> , 2019 , 23, e13364	1.8	4
349	Metabolomics for Investigating Physiological and Pathophysiological Processes. <i>Physiological Reviews</i> , 2019 , 99, 1819-1875	47.9	196
348	Urinary Organic Acids Increase After Clinical Stabilization of Hospitalized Children With Severe Acute Malnutrition. <i>Food and Nutrition Bulletin</i> , 2019 , 40, 532-543	1.8	
347	NMR metabolomics: A look ahead. <i>Journal of Magnetic Resonance</i> , 2019 , 306, 155-161	3	68
346	NMR Spectroscopy for Metabolomics Research. <i>Metabolites</i> , 2019 , 9,	5.6	330
345	Metabolomic profiling of the excretory-secretory products of hookworm and whipworm. <i>Metabolomics</i> , 2019 , 15, 101	4.7	16
344	Using MetaboAnalyst 4.0 for Comprehensive and Integrative Metabolomics Data Analysis. <i>Current Protocols in Bioinformatics</i> , 2019 , 68, e86	24.2	928
343	International Ring Trial of a High Resolution Targeted Metabolomics and Lipidomics Platform for Serum and Plasma Analysis. <i>Analytical Chemistry</i> , 2019 , 91, 14407-14416	7.8	42
342	The role of hydration effects in 5-fluorouridine binding to SOD1: insight from a new 3D-RISM-KH based protocol for including structural water in docking simulations. <i>Journal of Computer-Aided Molecular Design</i> , 2019 , 33, 913-926	4.2	4
341	Automated Tools for the Analysis of 1D-NMR and 2D-NMR Spectra. <i>Methods in Molecular Biology</i> , 2019 , 2037, 429-449	1.4	4
340	Solvent Composition Effects on the Structural Properties of the A β 2 Monomer from the 3D-RISM-KH Molecular Theory of Solvation. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 2491-2506	3.4	2

339	Impact of Bovine Diet on Metabolomic Profile of Skim Milk and Whey Protein Ingredients. <i>Metabolites</i> , 2019 , 9,	5.6	9
338	Assessing the performance of genome-wide association studies for predicting disease risk. <i>PLoS ONE</i> , 2019 , 14, e0220215	3.7	19
337	Nutrimetabolomics: An Integrative Action for Metabolomic Analyses in Human Nutritional Studies. <i>Molecular Nutrition and Food Research</i> , 2019 , 63, e1800384	5.9	107
336	Edible nuts deliver polyphenols and their transformation products to the large intestine: An in vitro fermentation model combining targeted/untargeted metabolomics. <i>Food Research International</i> , 2019 , 116, 786-794	7	31
335	CEU Mass Mediator 3.0: A Metabolite Annotation Tool. <i>Journal of Proteome Research</i> , 2019 , 18, 797-802	5.6	59
334	BioTransformer: a comprehensive computational tool for small molecule metabolism prediction and metabolite identification. <i>Journal of Cheminformatics</i> , 2019 , 11, 2	8.6	142
333	PHAST, PHASTER and PHASTEST: Tools for finding prophage in bacterial genomes. <i>Briefings in Bioinformatics</i> , 2019 , 20, 1560-1567	13.4	71
332	First-trimester metabolomic prediction of stillbirth. <i>Journal of Maternal-Fetal and Neonatal Medicine</i> , 2019 , 32, 3435-3441	2	4
331	Assessing the performance of genome-wide association studies for predicting disease risk 2019 , 14, e0220215		
330	Assessing the performance of genome-wide association studies for predicting disease risk 2019 , 14, e0220215		
329	Assessing the performance of genome-wide association studies for predicting disease risk 2019 , 14, e0220215		
328	Assessing the performance of genome-wide association studies for predicting disease risk 2019 , 14, e0220215		
327	Recommended strategies for spectral processing and post-processing of 1D H-NMR data of biofluids with a particular focus on urine. <i>Metabolomics</i> , 2018 , 14, 31	4.7	70
326	Guidelines for Biomarker of Food Intake Reviews (BFIRev): how to conduct an extensive literature search for biomarker of food intake discovery. <i>Genes and Nutrition</i> , 2018 , 13, 3	4.3	47
325	The role of the Human Metabolome Database in inborn errors of metabolism. <i>Journal of Inherited Metabolic Disease</i> , 2018 , 41, 329-336	5.4	9
324	DrugBank 5.0: a major update to the DrugBank database for 2018. <i>Nucleic Acids Research</i> , 2018 , 46, D1074-D1087	26.1	262
323	A sensitive, high-throughput LC-MS/MS method for measuring catecholamines in low volume serum. <i>Analytica Chimica Acta</i> , 2018 , 1037, 159-167	6.6	34
322	PAMDB: a comprehensive <i>Pseudomonas aeruginosa</i> metabolome database. <i>Nucleic Acids Research</i> , 2018 , 46, D575-D580	20.1	25

321	Evolution of renal function and urinary biomarker indicators of inflammation on serial kidney biopsies in pediatric kidney transplant recipients with and without rejection. <i>Pediatric Transplantation</i> , 2018 , 22, e13202	1.8	10
320	HMDB 4.0: the human metabolome database for 2018. <i>Nucleic Acids Research</i> , 2018 , 46, D608-D617	20.1	1832
319	Unraveling the unknown areas of the human metabolome: the role of infrared ion spectroscopy. <i>Journal of Inherited Metabolic Disease</i> , 2018 , 41, 367-377	5.4	32
318	Identification of serum metabolites associated with the risk of metritis in transition dairy cows. <i>Canadian Journal of Animal Science</i> , 2018 , 98, 525-537	0.9	5
317	nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. <i>Analytical Chemistry</i> , 2018 , 90, 649-656	7.8	37
316	Growth of Malignant Non-CNS Tumors Alters Brain Metabolome. <i>Frontiers in Genetics</i> , 2018 , 9, 41	4.5	2
315	Pasture Feeding Changes the Bovine Rumen and Milk Metabolome. <i>Metabolites</i> , 2018 , 8,	5.6	51
314	A review on human fecal metabolomics: Methods, applications and the human fecal metabolome database. <i>Analytica Chimica Acta</i> , 2018 , 1030, 1-24	6.6	111
313	CypReact: A Software Tool for in Silico Reactant Prediction for Human Cytochrome P450 Enzymes. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 1282-1291	6.1	31
312	Non-invasive staging of chronic kidney allograft damage using urine metabolomic profiling. <i>Pediatric Transplantation</i> , 2018 , 22, e13226	1.8	10
311	Rapid and reliable protein structure determination via chemical shift threading. <i>Journal of Biomolecular NMR</i> , 2018 , 70, 33-51	3	3
310	A Simple and Convenient Synthesis of Unlabeled and C-Labeled 3-(3-Hydroxyphenyl)-3-Hydroxypropionic Acid and Its Quantification in Human Urine Samples. <i>Metabolites</i> , 2018 , 8,	5.6	6
309	Non-invasive Point-of-Care Device To Diagnose Acute Mesenteric Ischemia. <i>ACS Sensors</i> , 2018 , 3, 2296-2302	3.02	5
308	A simple in vitro assay for assessing the efficacy, mechanisms and kinetics of anti-prion fibril compounds. <i>Prion</i> , 2018 , 12, 280-300	2.3	11
307	MetaboAnalyst 4.0: towards more transparent and integrative metabolomics analysis. <i>Nucleic Acids Research</i> , 2018 , 46, W486-W494	20.1	2157
306	Residue-specific mobility changes in soluble oligomers of the prion protein define regions involved in aggregation. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2018 , 1866, 982-988	4	2
305	Informatics and Data Analytics to Support Exposome-Based Discovery for Public Health. <i>Annual Review of Public Health</i> , 2017 , 38, 279-294	20.6	68
304	Metabotyping reveals distinct metabolic alterations in ketotic cows and identifies early predictive serum biomarkers for the risk of disease. <i>Metabolomics</i> , 2017 , 13, 1	4.7	25

303	Improved Glucose Homeostasis in Obese Mice Treated With Resveratrol Is Associated With Alterations in the Gut Microbiome. <i>Diabetes</i> , 2017 , 66, 418-425	0.9	121
302	Urinary Metabolomics for Noninvasive Detection of Antibody-Mediated Rejection in Children After Kidney Transplantation. <i>Transplantation</i> , 2017 , 101, 2553-2561	1.8	23
301	Targeted Metabolic Profiling of Post-Mortem Brain from Infants Who Died from Sudden Infant Death Syndrome. <i>Journal of Proteome Research</i> , 2017 , 16, 2587-2596	5.6	12
300	Microbiome and metabolome modifying effects of several cardiovascular disease interventions in apo-E mice. <i>Microbiome</i> , 2017 , 5, 30	16.6	55
299	Peptide-based fluorescence biosensors for detection/measurement of nanoparticles. <i>Analytical and Bioanalytical Chemistry</i> , 2017 , 409, 903-915	4.4	3
298	Exposome-Explorer: a manually-curated database on biomarkers of exposure to dietary and environmental factors. <i>Nucleic Acids Research</i> , 2017 , 45, D979-D984	20.1	77
297	The compound (3-{5-[(2,5-dimethoxyphenyl)amino]-1,3,4-thiadiazolidin-2-yl}-5,8-methoxy-2H-chromen-2-one) inhibits the prion protein conversion from PrP to PrP with lower IC in ScN2a cells. <i>Bioorganic and Medicinal Chemistry</i> , 2017 , 25, 5875-5888	3.4	2
296	Recombinant Incretin-Secreting Microbe Improves Metabolic Dysfunction in High-Fat Diet Fed Rodents. <i>Scientific Reports</i> , 2017 , 7, 13523	4.9	12
295	A scheme for a flexible classification of dietary and health biomarkers. <i>Genes and Nutrition</i> , 2017 , 12, 34	4.3	49
294	Development and Validation of a High-Throughput Mass Spectrometry Based Urine Metabolomic Test for the Detection of Colonic Adenomatous Polyps. <i>Metabolites</i> , 2017 , 7,	5.6	21
293	YMDB 2.0: a significantly expanded version of the yeast metabolome database. <i>Nucleic Acids Research</i> , 2017 , 45, D440-D445	20.1	83
292	DI/LC-MS/MS-Based Metabolic Profiling for Identification of Early Predictive Serum Biomarkers of Metritis in Transition Dairy Cows. <i>Journal of Agricultural and Food Chemistry</i> , 2017 , 65, 8510-8521	5.7	15
291	Unraveling the meaning of chemical shifts in protein NMR. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2017 , 1865, 1564-1576	4	17
290	A Web Tool for Generating High Quality Machine-readable Biological Pathways. <i>Journal of Visualized Experiments</i> , 2017 ,	1.6	3
289	Metallotyping of ketotic dairy cows reveals major alterations preceding, associating, and following the disease occurrence. <i>Metabolomics</i> , 2017 , 13, 1	4.7	4
288	Initial Structural Models of the A β 2 Dimer from Replica Exchange Molecular Dynamics Simulations. <i>ACS Omega</i> , 2017 , 2, 7621-7636	3.9	7
287	Combining traditional dietary assessment methods with novel metabolomics techniques: present efforts by the Food Biomarker Alliance. <i>Proceedings of the Nutrition Society</i> , 2017 , 76, 619-627	2.9	62
286	GC-MS Metabolomics Identifies Metabolite Alterations That Precede Subclinical Mastitis in the Blood of Transition Dairy Cows. <i>Journal of Proteome Research</i> , 2017 , 16, 433-446	5.6	41

285	Metabolomic determination of pathogenesis of late-onset preeclampsia. <i>Journal of Maternal-Fetal and Neonatal Medicine</i> , 2017 , 30, 658-664	2	20
284	The future of NMR-based metabolomics. <i>Current Opinion in Biotechnology</i> , 2017 , 43, 34-40	11.4	500
283	Livestock metabolomics and the livestock metabolome: A systematic review. <i>PLoS ONE</i> , 2017 , 12, e0177675	9.75	140
282	Dietary and metabolomic determinants of relapse in ulcerative colitis patients: A pilot prospective cohort study. <i>World Journal of Gastroenterology</i> , 2017 , 23, 3890-3899	5.6	16
281	Metabolomic prediction of endometrial cancer. <i>Metabolomics</i> , 2017 , 14, 6	4.7	15
280	Functionalized gold nanoparticle-enhanced competitive assay for sensitive small-molecule metabolite detection using surface plasmon resonance. <i>Analyst, The</i> , 2017 , 143, 289-296	5	26
279	ClassyFire: automated chemical classification with a comprehensive, computable taxonomy. <i>Journal of Cheminformatics</i> , 2016 , 8, 61	8.6	327
278	Nano-Optomechanical Systems for Gas Chromatography. <i>Nano Letters</i> , 2016 , 16, 6975-6981	11.5	15
277	SPLASH, a hashed identifier for mass spectra. <i>Nature Biotechnology</i> , 2016 , 34, 1099-1101	44.5	48
276	An impedance detection circuit for applications in a portable biosensor system 2016 ,		4
275	PHASTER: a better, faster version of the PHAST phage search tool. <i>Nucleic Acids Research</i> , 2016 , 44, W162-161	211	1573
274	Metabolic signatures of Huntington's disease (HD): (1)H NMR analysis of the polar metabolome in post-mortem human brain. <i>Biochimica Et Biophysica Acta - Molecular Basis of Disease</i> , 2016 , 1862, 1675-84	6.9	31
273	Introduction to Cheminformatics. <i>Current Protocols in Bioinformatics</i> , 2016 , 53, 14.1.1-14.1.21	24.2	10
272	Detecting Renal Allograft Inflammation Using Quantitative Urine Metabolomics and CXCL10. <i>Transplantation Direct</i> , 2016 , 2, e78	2.3	16
271	Clinical phenotype clustering in cardiovascular risk patients for the identification of responsive metabolotypes after red wine polyphenol intake. <i>Journal of Nutritional Biochemistry</i> , 2016 , 28, 114-20	6.3	44
270	ECMDB 2.0: A richer resource for understanding the biochemistry of E. coli. <i>Nucleic Acids Research</i> , 2016 , 44, D495-501	20.1	73
269	Identification of candidate biomarkers of brain damage in a mouse model of closed head injury: a metabolomic pilot study. <i>Metabolomics</i> , 2016 , 12, 1	4.7	13
268	Emerging applications of metabolomics in drug discovery and precision medicine. <i>Nature Reviews Drug Discovery</i> , 2016 , 15, 473-84	64.1	694

267	Recommendations and Standardization of Biomarker Quantification Using NMR-Based Metabolomics with Particular Focus on Urinary Analysis. <i>Journal of Proteome Research</i> , 2016 , 15, 360-73	5.6	94
266	Isolation of soluble scFv antibody fragments specific for small biomarker molecule, L-Carnitine, using phage display. <i>Journal of Immunological Methods</i> , 2016 , 428, 9-19	2.5	5
265	Cancer Metabolomics and the Human Metabolome Database. <i>Metabolites</i> , 2016 , 6,	5.6	84
264	Current and Future Perspectives on the Structural Identification of Small Molecules in Biological Systems. <i>Metabolites</i> , 2016 , 6,	5.6	84
263	Inter-Laboratory Robustness of Next-Generation Bile Acid Study in Mice and Humans: International Ring Trial Involving 12 Laboratories. <i>Journal of Applied Laboratory Medicine</i> , 2016 , 1, 129-142	2	20
262	Computational Prediction of Electron Ionization Mass Spectra to Assist in GC/MS Compound Identification. <i>Analytical Chemistry</i> , 2016 , 88, 7689-97	7.8	76
261	Using DrugBank for In Silico Drug Exploration and Discovery. <i>Current Protocols in Bioinformatics</i> , 2016 , 54, 14.4.1-14.4.31	24.2	22
260	Role of polysaccharide and lipid in lipopolysaccharide induced prion protein conversion. <i>Prion</i> , 2016 , 10, 466-483	2.3	5
259	Heatmapper: web-enabled heat mapping for all. <i>Nucleic Acids Research</i> , 2016 , 44, W147-53	20.1	957
258	Serum metabolomic markers for traumatic brain injury: a mouse model. <i>Metabolomics</i> , 2016 , 12, 1	4.7	17
257	Characterization of a highly potent antimicrobial peptide microcin N from uropathogenic <i>Escherichia coli</i> . <i>FEMS Microbiology Letters</i> , 2016 , 363,	2.9	6
256	Metabolomics enables precision medicine: "A White Paper, Community Perspective". <i>Metabolomics</i> , 2016 , 12, 149	4.7	327
255	Using MetaboAnalyst 3.0 for Comprehensive Metabolomics Data Analysis. <i>Current Protocols in Bioinformatics</i> , 2016 , 55, 14.10.1-14.10.91	24.2	957
254	Recombinant mouse prion protein alone or in combination with lipopolysaccharide alters expression of innate immunity genes in the colon of mice. <i>Prion</i> , 2015 , 9, 59-73	2.3	3
253	Accessible surface area from NMR chemical shifts. <i>Journal of Biomolecular NMR</i> , 2015 , 62, 387-401	3	8
252	Is Cancer a Genetic Disease or a Metabolic Disease?. <i>EBioMedicine</i> , 2015 , 2, 478-9	8.8	73
251	Simulating electrical properties of interdigitated electrode designs for impedance-based biosensing applications 2015 ,		1
250	Validation of metabolomic models for prediction of early-onset preeclampsia. <i>American Journal of Obstetrics and Gynecology</i> , 2015 , 213, 530.e1-530.e10	6.4	43

249	The human saliva metabolome. <i>Metabolomics</i> , 2015 , 11, 1864-1883	4.7	142
248	Metabolite profiling and expression analysis of flavonoid, vitamin C and tocopherol biosynthesis genes in the antioxidant-rich sea buckthorn (<i>Hippophae rhamnoides</i> L.). <i>Phytochemistry</i> , 2015 , 118, 181-91	4.1	27
247	In silico studies and fluorescence binding assays of potential anti-prion compounds reveal an important binding site for prion inhibition from PrP(C) to PrP(Sc). <i>European Journal of Medicinal Chemistry</i> , 2015 , 91, 118-31	6.8	9
246	Salmonella phages and prophages: genomics, taxonomy, and applied aspects. <i>Methods in Molecular Biology</i> , 2015 , 1225, 237-87	1.4	23
245	Competitive fragmentation modeling of ESI-MS/MS spectra for putative metabolite identification. <i>Metabolomics</i> , 2015 , 11, 98-110	4.7	237
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