

David I Broadhurst

List of Publications by Year in descending order

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Version: 2024-02-01

90
papers

14,974
citations

36299

51
h-index

45310

90
g-index

92
all docs

92
docs citations

92
times ranked

18494
citing authors

#	ARTICLE	IF	CITATIONS
1	Does machine learning have a role in the prediction of asthma in children?. Paediatric Respiratory Reviews, 2022, 41, 51-60.	1.8	8
2	Urinary metabolite of severe asthma evidences decreased carnitine metabolism independent of oral corticosteroid treatment in the U-BIOPRED study. European Respiratory Journal, 2022, 59, 2101733.	6.7	13
3	Improvement in the Prediction of Neonatal Hypoxic-Ischemic Encephalopathy with the Integration of Umbilical Cord Metabolites and Current Clinical Makers. Journal of Pediatrics, 2021, 229, 175-181.e1.	1.8	17
4	Extraction and quantitative determination of bile acids in feces. Analytica Chimica Acta, 2021, 1150, 338224.	5.4	17
5	Early and sustained Lactobacillus plantarum probiotic therapy in critical illness: the randomised, placebo-controlled, restoration of gut microflora in critical illness trial (ROCIT). Intensive Care Medicine, 2021, 47, 307-315.	8.2	22
6	Detecting Sex-Related Changes to the Metabolome of a Critically Endangered Freshwater Crayfish During the Mating Season. Frontiers in Molecular Biosciences, 2021, 8, 650839.	3.5	2
7	A strategy for advancing for population-based scientific discovery using the metabolome: the establishment of the Metabolomics Society Metabolomic Epidemiology Task Group. Metabolomics, 2021, 17, 45.	3.0	7
8	Data supporting development and validation of liquid chromatography tandem mass spectrometry method for the quantitative determination of bile acids in feces. Data in Brief, 2021, 36, 107091.	1.0	0
9	Kynurenic acid may underlie sex-specific immune responses to COVID-19. Science Signaling, 2021, 14, .	3.6	58
10	Sensitive and quantitative determination of short-chain fatty acids in human serum using liquid chromatography mass spectrometry. Analytical and Bioanalytical Chemistry, 2021, 413, 6333-6342.	3.7	22
11	Searching for a technology-driven acute rheumatic fever test: the START study protocol. BMJ Open, 2021, 11, e053720.	1.9	9
12	Dissemination and analysis of the quality assurance (QA) and quality control (QC) practices of LC-MS based untargeted metabolomics practitioners. Metabolomics, 2020, 16, 113.	3.0	56
13	Study protocol for the safety and efficacy of probiotic therapy on days alive and out of hospital in adult ICU patients: the multicentre, randomised, placebo-controlled Restoration Of gut microflora in Critical Illness Trial (ROCIT). BMJ Open, 2020, 10, e035930.	1.9	2
14	Migrating from partial least squares discriminant analysis to artificial neural networks: a comparison of functionally equivalent visualisation and feature contribution tools using jupyter notebooks. Metabolomics, 2020, 16, 17.	3.0	35
15	Notame Workflow for Non-Targeted LC-MS Metabolic Profiling. Metabolites, 2020, 10, 135.	2.9	71
16	The application of artificial neural networks in metabolomics: a historical perspective. Metabolomics, 2019, 15, 142.	3.0	66
17	A comparative evaluation of the generalised predictive ability of eight machine learning algorithms across ten clinical metabolomics data sets for binary classification. Metabolomics, 2019, 15, 150.	3.0	106
18	Does exercise impact gut microbiota composition in men receiving androgen deprivation therapy for prostate cancer? A single-blinded, two-armed, randomised controlled trial. BMJ Open, 2019, 9, e024872.	1.9	8

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19	Towards quality assurance and quality control in untargeted metabolomics studies. <i>Metabolomics</i> , 2019, 15, 4.	3.0	101
20	Characterizing the plasma metabolome during 14 days of live ^{high} , train ^{low} simulated altitude: A metabolomic approach. <i>Experimental Physiology</i> , 2019, 104, 81-92.	2.0	11
21	Untargeted metabolomic analysis and pathway discovery in perinatal asphyxia and hypoxic-ischaemic encephalopathy. <i>Journal of Cerebral Blood Flow and Metabolism</i> , 2019, 39, 147-162.	4.3	35
22	Toward collaborative open data science in metabolomics using Jupyter Notebooks and cloud computing. <i>Metabolomics</i> , 2019, 15, 125.	3.0	59
23	Comparison of computational approaches for identification and quantification of urinary metabolites in ¹ H NMR spectra. <i>Analytical Methods</i> , 2018, 10, 2129-2137.	2.7	4
24	OnPLS-Based Multi-Block Data Integration: A Multivariate Approach to Interrogating Biological Interactions in Asthma. <i>Analytical Chemistry</i> , 2018, 90, 13400-13408.	6.5	27
25	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.	3.0	517
26	Characterizing the plasma metabolome during and following a maximal exercise cycling test. <i>Journal of Applied Physiology</i> , 2018, 125, 1193-1203.	2.5	22
27	Preanalytical Processing and Biobanking Procedures of Biological Samples for Metabolomics Research: A White Paper, Community Perspective (for ^o Precision Medicine and Pharmacometabolomics) Tj ETQq1 0.784114 rgB	1.1	1
28	Quality assurance and quality control processes: summary of a metabolomics community questionnaire. <i>Metabolomics</i> , 2017, 13, 1.	3.0	53
29	Metabolomics enables precision medicine: ^o A White Paper, Community Perspective ^o . <i>Metabolomics</i> , 2016, 12, 149.	3.0	434
30	¹ H-NMR urinary metabolomic profiling for diagnosis of gastric cancer. <i>British Journal of Cancer</i> , 2016, 114, 59-62.	6.4	82
31	Metabolomics reveals the physiological response of <i>Pseudomonas putida</i> KT2440 (UWC1) after pharmaceutical exposure. <i>Molecular BioSystems</i> , 2016, 12, 1367-1377.	2.9	5
32	Reductions in circulating levels of IL-16, IL-7 and VEGF-A in myalgic encephalomyelitis/chronic fatigue syndrome. <i>Cytokine</i> , 2016, 78, 27-36.	3.2	40
33	Sildenafil Therapy Normalizes the Aberrant Metabolomic Profile in the Comt ^o / ^o Mouse Model of Preeclampsia/Fetal Growth Restriction. <i>Scientific Reports</i> , 2015, 5, 18241.	3.3	26
34	Exploring the mode of action of dithranol therapy for psoriasis: a metabolomic analysis using HaCaT cells. <i>Molecular BioSystems</i> , 2015, 11, 2198-2209.	2.9	20
35	Gestation ^o -specific ^o D ^o ^o dimer reference ranges: a cross ^o sectional study. <i>BJOG: an International Journal of Obstetrics and Gynaecology</i> , 2015, 122, 395-400.	2.3	66
36	Molecular phenotyping of a UK population: defining the human serum metabolome. <i>Metabolomics</i> , 2015, 11, 9-26.	3.0	202

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37	The effect of haemolysis on the metabolomic profile of umbilical cord blood. <i>Clinical Biochemistry</i> , 2015, 48, 534-537.	1.9	22
38	Macronutrient Regulation of Ghrelin and Peptide YY in Pediatric Obesity and Prader-Willi Syndrome. <i>Journal of Clinical Endocrinology and Metabolism</i> , 2015, 100, 3822-3831.	3.6	17
39	Direct infusion mass spectrometry metabolomics dataset: a benchmark for data processing and quality control. <i>Scientific Data</i> , 2014, 1, 140012.	5.3	134
40	Metabolomic profiling in multiple sclerosis: insights into biomarkers and pathogenesis. <i>Multiple Sclerosis Journal</i> , 2014, 20, 1396-1400.	3.0	80
41	The New Data Quality Task Group (DQTG): ensuring high quality data today and in the future. <i>Metabolomics</i> , 2014, 10, 539-540.	3.0	13
42	Rapid inflammasome activation in microglia contributes to brain disease in HIV/AIDS. <i>Retrovirology</i> , 2014, 11, 35.	2.0	180
43	On the Statistics of Identifying Candidate Pathogen Effectors. <i>Methods in Molecular Biology</i> , 2014, 1127, 53-64.	0.9	6
44	Evidence That Multiple Defects in Lipid Regulation Occur before Hyperglycemia during the Prodrome of Type-2 Diabetes. <i>PLoS ONE</i> , 2014, 9, e103217.	2.5	40
45	Translational biomarker discovery in clinical metabolomics: an introductory tutorial. <i>Metabolomics</i> , 2013, 9, 280-299.	3.0	765
46	¹ H NMR Derived Metabolomic Profile of Neonatal Asphyxia in Umbilical Cord Serum: Implications for Hypoxic Ischemic Encephalopathy. <i>Journal of Proteome Research</i> , 2013, 12, 4230-4239.	3.7	62
47	Characterising and correcting batch variation in an automated direct infusion mass spectrometry (DIMS) metabolomics workflow. <i>Analytical and Bioanalytical Chemistry</i> , 2013, 405, 5147-5157.	3.7	123
48	Angiogenic imbalance and plasma lipid alterations in women with preeclampsia from a developing country. <i>Growth Factors</i> , 2012, 30, 158-166.	1.7	14
49	Moving metabolomics from a data-driven science to an integrative systems science. <i>Genome Medicine</i> , 2012, 4, 85.	8.2	3
50	MetaboAnalyst 2.0--a comprehensive server for metabolomic data analysis. <i>Nucleic Acids Research</i> , 2012, 40, W127-W133.	14.5	1,058
51	The importance of experimental design and QC samples in large-scale and MS-driven untargeted metabolomic studies of humans. <i>Bioanalysis</i> , 2012, 4, 2249-2264.	1.5	382
52	Reference standard for serum bile acids in pregnancy. <i>BJOG: an International Journal of Obstetrics and Gynaecology</i> , 2012, 119, 493-498.	2.3	40
53	The Metabolomic Profile of Umbilical Cord Blood in Neonatal Hypoxic Ischaemic Encephalopathy. <i>PLoS ONE</i> , 2012, 7, e50520.	2.5	84
54	Systems level studies of mammalian metabolomes: the roles of mass spectrometry and nuclear magnetic resonance spectroscopy. <i>Chemical Society Reviews</i> , 2011, 40, 387-426.	38.1	689

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55	Procedures for large-scale metabolic profiling of serum and plasma using gas chromatography and liquid chromatography coupled to mass spectrometry. <i>Nature Protocols</i> , 2011, 6, 1060-1083.	12.0	2,236
56	Metabolic Profiling Uncovers a Phenotypic Signature of Small for Gestational Age in Early Pregnancy. <i>Journal of Proteome Research</i> , 2011, 10, 3660-3673.	3.7	99
57	Changes in the Metabolic Footprint of Placental Explant-Conditioned Medium Cultured in Different Oxygen Tensions from Placentas of Small for Gestational Age and Normal Pregnancies. <i>Placenta</i> , 2010, 31, 893-901.	1.5	55
58	Robust Early Pregnancy Prediction of Later Preeclampsia Using Metabolomic Biomarkers. <i>Hypertension</i> , 2010, 56, 741-749.	2.7	242
59	Biomarkers of Dietary Energy Restriction in Women at Increased Risk of Breast Cancer. <i>Cancer Prevention Research</i> , 2009, 2, 720-731.	1.5	41
60	Development and Performance of a Gas Chromatography- ² Time-of-Flight Mass Spectrometry Analysis for Large-Scale Nontargeted Metabolomic Studies of Human Serum. <i>Analytical Chemistry</i> , 2009, 81, 7038-7046.	6.5	168
61	Mass spectrometry tools and metabolite-specific databases for molecular identification in metabolomics. <i>Analyst</i> , 2009, 134, 1322.	3.5	240
62	Development of a Robust and Repeatable UPLC- ² MS Method for the Long-Term Metabolomic Study of Human Serum. <i>Analytical Chemistry</i> , 2009, 81, 1357-1364.	6.5	447
63	Changes in the Metabolic Footprint of Placental Explant-Conditioned Culture Medium Identifies Metabolic Disturbances Related to Hypoxia and Pre-Eclampsia. <i>Placenta</i> , 2009, 30, 974-980.	1.5	76
64	Metabolic profiling of serum using Ultra Performance Liquid Chromatography and the LTQ-Orbitrap mass spectrometry system. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2008, 871, 288-298.	2.3	161
65	Global Metabolic Profiling of <i>Escherichia coli</i> Cultures: an Evaluation of Methods for Quenching and Extraction of Intracellular Metabolites. <i>Analytical Chemistry</i> , 2008, 80, 2939-2948.	6.5	293
66	Detection and Identification of Novel Metabolomic Biomarkers in Preeclampsia. <i>Reproductive Sciences</i> , 2008, 15, 591-597.	2.5	84
67	A GC-TOF-MS study of the stability of serum and urine metabolomes during the UK Biobank sample collection and preparation protocols. <i>International Journal of Epidemiology</i> , 2008, 37, i23-i30.	1.9	118
68	Closed-Loop, Multiobjective Optimization of Two-Dimensional Gas Chromatography/Mass Spectrometry for Serum Metabolomics. <i>Analytical Chemistry</i> , 2007, 79, 464-476.	6.5	94
69	Growth control of the eukaryote cell: a systems biology study in yeast. <i>Journal of Biology</i> , 2007, 6, 4.	2.7	234
70	Soil differentiation using fingerprint Fourier transform infrared spectroscopy, chemometrics and genetic algorithm-based feature selection. <i>Soil Biology and Biochemistry</i> , 2007, 39, 2888-2896.	8.8	48
71	Statistical strategies for avoiding false discoveries in metabolomics and related experiments. <i>Metabolomics</i> , 2007, 2, 171-196.	3.0	658
72	Serum metabolomics reveals many novel metabolic markers of heart failure, including pseudouridine and 2-oxoglutarate. <i>Metabolomics</i> , 2007, 3, 413-426.	3.0	150

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73	Proposed minimum reporting standards for data analysis in metabolomics. <i>Metabolomics</i> , 2007, 3, 231-241.	3.0	361
74	Huntington disease patients and transgenic mice have similar pro-catabolic serum metabolite profiles. <i>Brain</i> , 2006, 129, 877-886.	7.6	175
75	Using metabolic fingerprinting of plants for evaluating nitrogen deposition impacts on the landscape level. <i>Global Change Biology</i> , 2006, 12, 1460-1465.	9.5	22
76	PYCHEM: a multivariate analysis package for python. <i>Bioinformatics</i> , 2006, 22, 2565-2566.	4.1	75
77	Differentiation of Peats Used in the Preparation of Malt for Scotch Whisky Production Using Fourier Transform Infrared Spectroscopy. <i>Journal of the Institute of Brewing</i> , 2006, 112, 333-339.	2.3	14
78	A laser desorption ionisation mass spectrometry approach for high throughput metabolomics. <i>Metabolomics</i> , 2005, 1, 243-250.	3.0	27
79	Rapid identification of closely related muscle foods by vibrational spectroscopy and machine learning. <i>Analyst</i> , The, 2005, 130, 1648.	3.5	109
80	Rapid and quantitative detection of the microbial spoilage of beef by Fourier transform infrared spectroscopy and machine learning. <i>Analytica Chimica Acta</i> , 2004, 514, 193-201.	5.4	119
81	Discrimination of Modes of Action of Antifungal Substances by Use of Metabolic Footprinting. <i>Applied and Environmental Microbiology</i> , 2004, 70, 6157-6165.	3.1	73
82	High-Throughput Metabolic Fingerprinting of Legume Silage Fermentations via Fourier Transform Infrared Spectroscopy and Chemometrics. <i>Applied and Environmental Microbiology</i> , 2004, 70, 1583-1592.	3.1	52
83	Functional Genomics via Metabolic Footprinting: Monitoring Metabolite Secretion by <i>Escherichia coli</i> Tryptophan Metabolism Mutants Using FT-IR and Direct Injection Electrospray Mass Spectrometry. <i>Comparative and Functional Genomics</i> , 2003, 4, 376-391.	2.0	110
84	Metabolic fingerprinting of salt-stressed tomatoes. <i>Phytochemistry</i> , 2003, 62, 919-928.	2.9	210
85	High-throughput classification of yeast mutants for functional genomics using metabolic footprinting. <i>Nature Biotechnology</i> , 2003, 21, 692-696.	17.5	500
86	Explanatory Optimization of Protein Mass Spectrometry via Genetic Search. <i>Analytical Chemistry</i> , 2003, 75, 6679-6686.	6.5	39
87	Rapid and Quantitative Detection of the Microbial Spoilage of Meat by Fourier Transform Infrared Spectroscopy and Machine Learning. <i>Applied and Environmental Microbiology</i> , 2002, 68, 2822-2828.	3.1	281
88	Monitoring of complex industrial bioprocesses for metabolite concentrations using modern spectroscopies and machine learning: Application to gibberellic acid production. <i>Biotechnology and Bioengineering</i> , 2002, 78, 527-538.	3.3	79
89	A functional genomics strategy that uses metabolome data to reveal the phenotype of silent mutations. <i>Nature Biotechnology</i> , 2001, 19, 45-50.	17.5	948
90	Genetic algorithms as a method for variable selection in multiple linear regression and partial least squares regression, with applications to pyrolysis mass spectrometry. <i>Analytica Chimica Acta</i> , 1997, 348, 71-86.	5.4	259