

# David I Broadhurst

## List of Publications by Year in descending order

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90  
papers

14,974  
citations

36303

51  
h-index

45317

90  
g-index

92  
all docs

92  
docs citations

92  
times ranked

18494  
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	MetaboAnalyst 2.0--a comprehensive server for metabolomic data analysis. <i>Nucleic Acids Research</i> , 2012, 40, W127-W133.	14.5	1,058
3	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
4	Translational biomarker discovery in clinical metabolomics: an introductory tutorial. <i>Metabolomics</i> , 2013, 9, 280-299.	3.0	765
5	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
6	Statistical strategies for avoiding false discoveries in metabolomics and related experiments. <i>Metabolomics</i> , 2007, 2, 171-196.	3.0	658
7	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
8	High-throughput classification of yeast mutants for functional genomics using metabolic footprinting. <i>Nature Biotechnology</i> , 2003, 21, 692-696.	17.5	500
9	Development of a Robust and Repeatable UPLC-MS Method for the Long-Term Metabolomic Study of Human Serum. <i>Analytical Chemistry</i> , 2009, 81, 1357-1364.	6.5	447
10	Metabolomics enables precision medicine: "A White Paper, Community Perspective". <i>Metabolomics</i> , 2016, 12, 149.	3.0	434
11	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
12	Proposed minimum reporting standards for data analysis in metabolomics. <i>Metabolomics</i> , 2007, 3, 231-241.	3.0	361
13	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
14	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
15	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
16	Robust Early Pregnancy Prediction of Later Preeclampsia Using Metabolomic Biomarkers. <i>Hypertension</i> , 2010, 56, 741-749.	2.7	242
17	Mass spectrometry tools and metabolite-specific databases for molecular identification in metabolomics. <i>Analyst</i> , 2009, 134, 1322.	3.5	240
18	Growth control of the eukaryote cell: a systems biology study in yeast. <i>Journal of Biology</i> , 2007, 6, 4.	2.7	234

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19	Metabolic fingerprinting of salt-stressed tomatoes. <i>Phytochemistry</i> , 2003, 62, 919-928.	2.9	210
20	Molecular phenotyping of a UK population: defining the human serum metabolome. <i>Metabolomics</i> , 2015, 11, 9-26.	3.0	202
21	Rapid inflammasome activation in microglia contributes to brain disease in HIV/AIDS. <i>Retrovirology</i> , 2014, 11, 35.	2.0	180
22	Huntington disease patients and transgenic mice have similar pro-catabolic serum metabolite profiles. <i>Brain</i> , 2006, 129, 877-886.	7.6	175
23	Development and Performance of a Gas Chromatography~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
24	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
25	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
26	Direct infusion mass spectrometry metabolomics dataset: a benchmark for data processing and quality control. <i>Scientific Data</i> , 2014, 1, 140012.	5.3	134
27	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
28	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
29	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
30	Preanalytical Processing and Biobanking Procedures of Biological Samples for Metabolomics Research: A White Paper, Community Perspective (for ~Precision Medicine and Pharmacometabolomics) Tj ETQq20 0 rgBT1/O	0.0	0
31	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
32	Rapid identification of closely related muscle foods by vibrational spectroscopy and machine learning. <i>Analyst</i> , The, 2005, 130, 1648.	3.5	109
33	A comparative evaluation of the generalised predictive ability of eight machine learning algorithms across ten clinical metabolomics data sets for binary classification. <i>Metabolomics</i> , 2019, 15, 150.	3.0	106
34	Towards quality assurance and quality control in untargeted metabolomics studies. <i>Metabolomics</i> , 2019, 15, 4.	3.0	101
35	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
36	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

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37	Detection and Identification of Novel Metabolomic Biomarkers in Preeclampsia. <i>Reproductive Sciences</i> , 2008, 15, 591-597.	2.5	84
38	The Metabolomic Profile of Umbilical Cord Blood in Neonatal Hypoxic Ischaemic Encephalopathy. <i>PLoS ONE</i> , 2012, 7, e50520.	2.5	84
39	<sup>1</sup> H-NMR urinary metabolomic profiling for diagnosis of gastric cancer. <i>British Journal of Cancer</i> , 2016, 114, 59-62.	6.4	82
40	Metabolomic profiling in multiple sclerosis: insights into biomarkers and pathogenesis. <i>Multiple Sclerosis Journal</i> , 2014, 20, 1396-1400.	3.0	80
41	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
42	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
43	PYCHEM: a multivariate analysis package for python. <i>Bioinformatics</i> , 2006, 22, 2565-2566.	4.1	75
44	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
45	Notame Workflow for Non-Targeted LC-MS Metabolic Profiling. <i>Metabolites</i> , 2020, 10, 135.	2.9	71
46	Gestation-specific D-dimer reference ranges: a cross-sectional study. <i>BJOG: an International Journal of Obstetrics and Gynaecology</i> , 2015, 122, 395-400.	2.3	66
47	The application of artificial neural networks in metabolomics: a historical perspective. <i>Metabolomics</i> , 2019, 15, 142.	3.0	66
48	<sup>1</sup> 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
49	Toward collaborative open data science in metabolomics using Jupyter Notebooks and cloud computing. <i>Metabolomics</i> , 2019, 15, 125.	3.0	59
50	Kynurenic acid may underlie sex-specific immune responses to COVID-19. <i>Science Signaling</i> , 2021, 14, .	3.6	58
51	Dissemination and analysis of the quality assurance (QA) and quality control (QC) practices of LC-MS based untargeted metabolomics practitioners. <i>Metabolomics</i> , 2020, 16, 113.	3.0	56
52	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
53	Quality assurance and quality control processes: summary of a metabolomics community questionnaire. <i>Metabolomics</i> , 2017, 13, 1.	3.0	53
54	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

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55	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
56	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
57	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
58	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
59	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
60	Explanatory Optimization of Protein Mass Spectrometry via Genetic Search. <i>Analytical Chemistry</i> , 2003, 75, 6679-6686.	6.5	39
61	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
62	Migrating from partial least squares discriminant analysis to artificial neural networks: a comparison of functionally equivalent visualisation and feature contribution tools using jupyter notebooks. <i>Metabolomics</i> , 2020, 16, 17.	3.0	35
63	A laser desorption ionisation mass spectrometry approach for high throughput metabolomics. <i>Metabolomics</i> , 2005, 1, 243-250.	3.0	27
64	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
65	Sildenafil Therapy Normalizes the Aberrant Metabolomic Profile in the Comtâ~/â~ Mouse Model of Preeclampsia/Fetal Growth Restriction. <i>Scientific Reports</i> , 2015, 5, 18241.	3.3	26
66	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
67	The effect of haemolysis on the metabolomic profile of umbilical cord blood. <i>Clinical Biochemistry</i> , 2015, 48, 534-537.	1.9	22
68	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
69	Early and sustained <i>Lactobacillus plantarum</i> probiotic therapy in critical illness: the randomised, placebo-controlled, restoration of gut microflora in critical illness trial (ROCIT). <i>Intensive Care Medicine</i> , 2021, 47, 307-315.	8.2	22
70	Sensitive and quantitative determination of short-chain fatty acids in human serum using liquid chromatography mass spectrometry. <i>Analytical and Bioanalytical Chemistry</i> , 2021, 413, 6333-6342.	3.7	22
71	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
72	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

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73	Improvement in the Prediction of Neonatal Hypoxic-Ischemic Encephalopathy with the Integration of Umbilical Cord Metabolites and Current Clinical Makers. <i>Journal of Pediatrics</i> , 2021, 229, 175-181.e1.	1.8	17
74	Extraction and quantitative determination of bile acids in feces. <i>Analytica Chimica Acta</i> , 2021, 1150, 338224.	5.4	17
75	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
76	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
77	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
78	Urinary metabotype of severe asthma evidences decreased carnitine metabolism independent of oral corticosteroid treatment in the U-BIOPRED study. <i>European Respiratory Journal</i> , 2022, 59, 2101733.	6.7	13
79	Characterizing the plasma metabolome during 14 days of live <sup>high</sup> , train <sup>low</sup> simulated altitude: A metabolomic approach. <i>Experimental Physiology</i> , 2019, 104, 81-92.	2.0	11
80	Searching for a technology-driven acute rheumatic fever test: the START study protocol. <i>BMJ Open</i> , 2021, 11, e053720.	1.9	9
81	Does exercise impact gut microbiota composition in men receiving androgen deprivation therapy for prostate cancer? A single-blinded, two-armed, randomised controlled trial. <i>BMJ Open</i> , 2019, 9, e024872.	1.9	8
82	Does machine learning have a role in the prediction of asthma in children?. <i>Paediatric Respiratory Reviews</i> , 2022, 41, 51-60.	1.8	8
83	A strategy for advancing for population-based scientific discovery using the metabolome: the establishment of the Metabolomics Society Metabolomic Epidemiology Task Group. <i>Metabolomics</i> , 2021, 17, 45.	3.0	7
84	On the Statistics of Identifying Candidate Pathogen Effectors. <i>Methods in Molecular Biology</i> , 2014, 1127, 53-64.	0.9	6
85	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
86	Comparison of computational approaches for identification and quantification of urinary metabolites in <sup>1</sup> H NMR spectra. <i>Analytical Methods</i> , 2018, 10, 2129-2137.	2.7	4
87	Moving metabolomics from a data-driven science to an integrative systems science. <i>Genome Medicine</i> , 2012, 4, 85.	8.2	3
88	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). <i>BMJ Open</i> , 2020, 10, e035930.	1.9	2
89	Detecting Sex-Related Changes to the Metabolome of a Critically Endangered Freshwater Crayfish During the Mating Season. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 650839.	3.5	2
90	Data supporting development and validation of liquid chromatography tandem mass spectrometry method for the quantitative determination of bile acids in feces. <i>Data in Brief</i> , 2021, 36, 107091.	1.0	0