Timothy Ebbels

List of Publications by Year in Descending Order

134 papers	9,422 citations	48 h-index	96 g-index
151 ext. papers	10,683 ext. citations	6.1 avg, IF	5.64 L-index

#	Paper	IF	Citations
134	Blood pressure interactions with the DASH dietary pattern, sodium, and potassium: The International Study of Macro-/Micronutrients and Blood Pressure (INTERMAP).. *American Journal of Clinical Nutrition*, **2022**,	7	1
133	Metabolomics: The Stethoscope for the Twenty-First Century. *Medical Principles and Practice*, **2021**, 30, 301-310	2.1	17
132	Bayesian Deconvolution and Quantification of Metabolites from J-Resolved NMR Spectroscopy. *Bayesian Analysis*, **2021**, 16,	2.3	1
131	Multiple-testing correction in metabolome-wide association studies. *BMC Bioinformatics*, **2021**, 22, 67	3.6	1
130	Statistical analysis in metabolic phenotyping. *Nature Protocols*, **2021**, 16, 4299-4326	18.8	8
129	Pathway analysis in metabolomics: Recommendations for the use of over-representation analysis. *PLoS Computational Biology*, **2021**, 17, e1009105	5	4
128	Progress towards an OECD reporting framework for transcriptomics and metabolomics in regulatory toxicology. *Regulatory Toxicology and Pharmacology*, **2021**, 125, 105020	3.4	6
127	Extraction and Integration of Genetic Networks from Short-Profile Omic Data Sets. *Metabolites*, **2020**, 10,	5.6	2
126	Targeted realignment of LC-MS profiles by neighbor-wise compound-specific graphical time warping with misalignment detection. *Bioinformatics*, **2020**, 36, 2862-2871	7.2	5
125	Integrative analysis of time course metabolic data and biomarker discovery. *BMC Bioinformatics*, **2020**, 21, 11	3.6	4
124	The association of fish consumption and its urinary metabolites with cardiovascular risk factors: the International Study of Macro-/Micronutrients and Blood Pressure (INTERMAP). *American Journal of Clinical Nutrition*, **2020**, 111, 280-290	7	18
123	Comparison of Bi- and Tri-Linear PLS Models for Variable Selection in Metabolomic Time-Series Experiments. *Metabolites*, **2019**, 9,	5.6	2
122	Serum metabolic signatures of coronary and carotid atherosclerosis and subsequent cardiovascular disease. *European Heart Journal*, **2019**, 40, 2883-2896	9.5	58
121	Data mining and visualisation: general discussion. *Faraday Discussions*, **2019**, 218, 354-371	3.6	2
120	Use cases, best practice and reporting standards for metabolomics in regulatory toxicology. *Nature Communications*, **2019**, 10, 3041	17.4	62
119	Predictive modelling using pathway scores: robustness and significance of pathway collections. *BMC Bioinformatics*, **2019**, 20, 543	3.6	8
118	Statistical Methods in Metabolomics **2019**, 949-976		1

117	Processing and Analysis of Untargeted Multicohort NMR Data. *Methods in Molecular Biology*, **2019**, 2037, 453-470	1.4	2
116	PhenoMeNal: processing and analysis of metabolomics data in the cloud. *GigaScience*, **2019**, 8,	7.6	41
115	Big Data and Databases for Metabolic Phenotyping **2019**, 329-367		2
114	Optimized Phenotypic Biomarker Discovery and Confounder Elimination via Covariate-Adjusted Projection to Latent Structures from Metabolic Spectroscopy Data. *Journal of Proteome Research*, **2018**, 17, 1586-1595	5.6	20
113	A comparison of human serum and plasma metabolites using untargeted H NMR spectroscopy and UPLC-MS. *Metabolomics*, **2018**, 14, 32	4.7	20
112	nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. *Analytical Chemistry*, **2018**, 90, 649-656	7.8	37
111	Bayesian estimation of the number of protonation sites for urinary metabolites from NMR spectroscopic data. *Metabolomics*, **2018**, 14, 56	4.7	2
110	Reliability of plasma polar metabolite concentrations in a large-scale cohort study using capillary electrophoresis-mass spectrometry. *PLoS ONE*, **2018**, 13, e0191230	3.7	40
109	CHAPTER 12:Advances in Computational Analysis of Metabolomic NMR Data. *New Developments in NMR*, **2018**, 310-323	0.9	1
108	Computational tools and workflows in metabolomics: An international survey highlights the opportunity for harmonisation through Galaxy. *Metabolomics*, **2017**, 13, 12	4.7	52
107	Metabolic phenotyping for discovery of urinary biomarkers of diet, xenobiotics and blood pressure in the INTERMAP Study: an overview. *Hypertension Research*, **2017**, 40, 336-345	4.7	12
106	Applying 'omics technologies in chemicals risk assessment: Report of an ECETOC workshop. *Regulatory Toxicology and Pharmacology*, **2017**, 91 Suppl 1, S3-S13	3.4	74
105	Framework for the quality assurance of 'omics technologies considering GLP requirements. *Regulatory Toxicology and Pharmacology*, **2017**, 91 Suppl 1, S27-S35	3.4	20
104	Improving Visualization and Interpretation of Metabolome-Wide Association Studies: An Application in a Population-Based Cohort Using Untargeted H NMR Metabolic Profiling. *Journal of Proteome Research*, **2017**, 16, 3623-3633	5.6	17
103	Bayesian inference for multiple Gaussian graphical models with application to metabolic association networks. *Annals of Applied Statistics*, **2017**, 11,	2.1	18
102	The future of metabolomics in ELIXIR. *F1000Research*, **2017**, 6,	3.6	18
101	The future of metabolomics in ELIXIR. *F1000Research*, **2017**, 6, 1649	3.6	10
100	Modelling the acid/base H NMR chemical shift limits of metabolites in human urine. *Metabolomics*, **2016**, 12, 152	4.7	24

99	Workflow for Integrated Processing of Multicohort Untargeted H NMR Metabolomics Data in Large-Scale Metabolic Epidemiology. *Journal of Proteome Research*, **2016**, 15, 4188-4194	5.6	28
98	Data standards can boost metabolomics research, and if there is a will, there is a way. *Metabolomics* , **2016**, 12, 14	4.7	85
97	Statistical Correlations between NMR Spectroscopy and Direct Infusion FT-ICR Mass Spectrometry Aid Annotation of Unknowns in Metabolomics. *Analytical Chemistry*, **2016**, 88, 2583-9	7.8	20
96	Synergistic and Antagonistic Mutation Responses of Human MCL-5 Cells to Mixtures of Benzo[a]pyrene and 2-Amino-1-Methyl-6-Phenylimidazo[4,5-b]pyridine: Dose-Related Variation in the Joint Effects of Common Dietary Carcinogens. *Environmental Health Perspectives*, **2016**, 124, 88-96	8.4	21
95	Urinary hippurate and proline betaine relative to fruit intake, blood pressure, and body mass index. *Proceedings of the Nutrition Society*, **2016**, 75,	2.9	1
94	Power Analysis and Sample Size Determination in Metabolic Phenotyping. *Analytical Chemistry*, **2016**, 88, 5179-88	7.8	70
93	Over-representation of correlation analysis (ORCA): a method for identifying associations between variable sets. *Bioinformatics*, **2015**, 31, 102-8	7.2	2
92	Urinary metabolic signatures of human adiposity. *Science Translational Medicine*, **2015**, 7, 285ra62	17.5	141
91	Embedding standards in metabolomics: the Metabolomics Society data standards task group. *Metabolomics*, **2015**, 11, 782-783	4.7	12
90	COordination of Standards in MetabOlomicS (COSMOS): facilitating integrated metabolomics data access. *Metabolomics*, **2015**, 11, 1587-1597	4.7	109
89	diXa: a data infrastructure for chemical safety assessment. *Bioinformatics*, **2015**, 31, 1505-7	7.2	27
88	Identifying biochemical phenotypic differences between cryptic species. *Biology Letters*, **2014**, 10,	3.6	12
87	Bayesian deconvolution and quantification of metabolites in complex 1D NMR spectra using BATMAN. *Nature Protocols*, **2014**, 9, 1416-27	18.8	132
86	Design and analysis of metabolomics studies in epidemiologic research: a primer on -omic technologies. *American Journal of Epidemiology*, **2014**, 180, 129-39	3.8	123
85	Genome metabolome integrated network analysis to uncover connections between genetic variants and complex traits: an application to obesity. *Journal of the Royal Society Interface*, **2014**, 11, 20130908	4.1	18
84	Orders of magnitude extension of the effective dynamic range of TDC-based TOFMS data through maximum likelihood estimation. *Journal of the American Society for Mass Spectrometry*, **2014**, 25, 1824-7	3.5	4
83	Variance and covariance heterogeneity analysis for detection of metabolites associated with cadmium exposure. *Statistical Applications in Genetics and Molecular Biology*, **2014**, 13, 191-201	1.2	4
82	1H NMR-based profiling reveals differential immune-metabolic networks during influenza virus infection in obese mice. *PLoS ONE*, **2014**, 9, e97238	3.7	20

81	Proteomic and metabolomic responses to connexin43 silencing in primary hepatocyte cultures. *Archives of Toxicology*, **2013**, 87, 883-94	5.8	10
80	Report on the 9th Annual International Conference of the Metabolomics Society. *Metabolomics*, **2013**, 9, 935-937	4.7	
79	A combination of transcriptomics and metabolomics uncovers enhanced bile acid biosynthesis in HepG2 cells expressing CCAAT/enhancer-binding protein [(C/EBP)], hepatocyte nuclear factor 4 (HNF4)], and constitutive androstane receptor (CAR). *Journal of Proteome Research*, **2013**, 12, 2732-41	5.6	5
78	Combining spectral ordering with peak fitting for one-dimensional NMR quantitative metabolomics. *Analytical Chemistry*, **2013**, 85, 4605-12	7.8	18
77	Integrated histopathological and urinary metabonomic investigation of the pathogenesis of microcystin-LR toxicosis. *Veterinary Pathology*, **2013**, 50, 159-71	2.8	13
76	Dietary and urinary metabonomic factors possibly accounting for higher blood pressure of black compared with white Americans: results of International Collaborative Study on macro-/micronutrients and blood pressure. *Hypertension*, **2013**, 62, 1074-80	8.5	22
75	Untargeted metabolome quantitative trait locus mapping associates variation in urine glycerate to mutant glycerate kinase. *Journal of Proteome Research*, **2012**, 11, 631-42	5.6	23
74	BATMAN--an R package for the automated quantification of metabolites from nuclear magnetic resonance spectra using a Bayesian model. *Bioinformatics*, **2012**, 28, 2088-90	7.2	118
73	A Bayesian Model of NMR Spectra for the Deconvolution and Quantification of Metabolites in Complex Biological Mixtures. *Journal of the American Statistical Association*, **2012**, 107, 1259-1271	2.8	34
72	Intra- and interlaboratory reproducibility of ultra performance liquid chromatography-time-of-flight mass spectrometry for urinary metabolic profiling. *Analytical Chemistry*, **2012**, 84, 2424-32	7.8	36
71	Subset optimization by reference matching (STORM): an optimized statistical approach for recovery of metabolic biomarker structural information from 1H NMR spectra of biofluids. *Analytical Chemistry*, **2012**, 84, 10694-701	7.8	64
70	Optimizing the use of quality control samples for signal drift correction in large-scale urine metabolic profiling studies. *Analytical Chemistry*, **2012**, 84, 2670-7	7.8	104
69	Characterization of data analysis methods for information recovery from metabolic 1H NMR spectra using artificial complex mixtures. *Metabolomics*, **2012**, 8, 1170-1180	4.7	3
68	Prospects for a statistical theory of LC/TOFMS data. *Journal of the American Society for Mass Spectrometry*, **2012**, 23, 779-91	3.5	3
67	Statistical Data Analysis in Metabolomics **2011**, 163-180		2
66	Optimized preprocessing of ultra-performance liquid chromatography/mass spectrometry urinary metabolic profiles for improved information recovery. *Analytical Chemistry*, **2011**, 83, 5864-72	7.8	201
65	Data-driven approach for metabolite relationship recovery in biological 1H NMR data sets using iterative statistical total correlation spectroscopy. *Analytical Chemistry*, **2011**, 83, 2075-82	7.8	35
64	Metabolic response to low-level toxicant exposure in a novel renal tubule epithelial cell system. *Molecular BioSystems*, **2011**, 7, 247-57		48

63	Response to Comment on "Optimized Preprocessing of Ultra-Performance Liquid Chromatography/Mass Spectrometry Urinary Metabolic Profiles for Improved Information Recovery" *Analytical Chemistry*, **2011**, 83, 9721-9722	7.8	2
62	A statistical framework for biomarker discovery in metabolomic time course data. *Bioinformatics*, **2011**, 27, 1979-85	7.2	36
61	Modelling short time series in metabolomics: a functional data analysis approach. *Advances in Experimental Medicine and Biology*, **2011**, 696, 307-15	3.6	11
60	Meeting-in-the-middle using metabolic profiling - a strategy for the identification of intermediate biomarkers in cohort studies. *Biomarkers*, **2011**, 16, 83-8	2.6	88
59	Consensus-phenotype integration of transcriptomic and metabolomic data implies a role for metabolism in the chemosensitivity of tumour cells. *PLoS Computational Biology*, **2011**, 7, e1001113	5	65
58	Integrated pathway-level analysis of transcriptomics and metabolomics data with IMPaLA. *Bioinformatics*, **2011**, 27, 2917-8	7.2	239
57	A differential network approach to exploring differences between biological states: an application to prediabetes. *PLoS ONE*, **2011**, 6, e24702	3.7	27
56	Processing and modeling of nuclear magnetic resonance (NMR) metabolic profiles. *Methods in Molecular Biology*, **2011**, 708, 365-88	1.4	23
55	High-resolution magic-angle-spinning NMR spectroscopy for metabolic profiling of intact tissues. *Nature Protocols*, **2010**, 5, 1019-32	18.8	309
54	Metabolome-wide association study identifies multiple biomarkers that discriminate north and south Chinese populations at differing risks of cardiovascular disease: INTERMAP study. *Journal of Proteome Research*, **2010**, 9, 6647-54	5.6	106
53	Bidirectional correlation of NMR and capillary electrophoresis fingerprints: a new approach to investigating Schistosoma mansoni infection in a mouse model. *Analytical Chemistry*, **2010**, 82, 203-10	7.8	27
52	A statistically rigorous test for the identification of parent-fragment pairs in LC-MS datasets. *Analytical Chemistry*, **2010**, 82, 1766-78	7.8	21
51	Effect of the histone deacetylase inhibitor trichostatin a on the metabolome of cultured primary hepatocytes. *Journal of Proteome Research*, **2010**, 9, 413-9	5.6	12
50	Construction of confidence regions for isotopic abundance patterns in LC/MS data sets for rigorous determination of molecular formulas. *Analytical Chemistry*, **2010**, 82, 7319-28	7.8	9
49	NMR-based metabolic profiling identifies biomarkers of liver regeneration following partial hepatectomy in the rat. *Journal of Proteome Research*, **2010**, 9, 59-69	5.6	68
48	A combined metabonomic and transcriptomic approach to investigate metabolism during development in the chick chorioallantoic membrane. *Journal of Proteome Research*, **2010**, 9, 3126-34	5.6	12
47	Opening up the "Black Box": metabolic phenotyping and metabolome-wide association studies in epidemiology. *Journal of Clinical Epidemiology*, **2010**, 63, 970-9	5.7	113
46	Optimization and evaluation of metabolite extraction protocols for untargeted metabolic profiling of liver samples by UPLC-MS. *Analytical Chemistry*, **2010**, 82, 7779-86	7.8	144

45	Correction of mass calibration gaps in liquid chromatography-mass spectrometry metabolomics data. *Bioinformatics*, **2010**, 26, 2488-9	7.2	119
44	Metabolic profiling and the metabolome-wide association study: significance level for biomarker identification. *Journal of Proteome Research*, **2010**, 9, 4620-7	5.6	102
43	MetAssimulo: simulation of realistic NMR metabolic profiles. *BMC Bioinformatics*, **2010**, 11, 496	3.6	17
42	The evolution of partial least squares models and related chemometric approaches in metabonomics and metabolic phenotyping. *Journal of Chemometrics*, **2010**, 24, 636-649	1.6	104
41	Intra- and inter-omic fusion of metabolic profiling data in a systems biology framework. *Chemometrics and Intelligent Laboratory Systems*, **2010**, 104, 121-131	3.8	48
40	Correlation Network Analysis reveals a sequential reorganization of metabolic and transcriptional states during germination and gene-metabolite relationships in developing seedlings of Arabidopsis. *BMC Systems Biology*, **2010**, 4, 62	3.5	41
39	Genetic algorithms for simultaneous variable and sample selection in metabonomics. *Bioinformatics* , **2009**, 25, 112-8	7.2	50
38	Time-resolved metabolic footprinting for nonlinear modeling of bacterial substrate utilization. *Applied and Environmental Microbiology*, **2009**, 75, 2453-63	4.8	46
37	Metabonomic investigations into the global biochemical sequelae of exposure to the pancreatic toxin 1-cyano-2-hydroxy-3-butene in the rat. *Magnetic Resonance in Chemistry*, **2009**, 47 Suppl 1, S26-35	2.1	12
36	Validation of metabolomics for toxic mechanism of action screening with the earthworm Lumbricus rubellus. *Metabolomics*, **2009**, 5, 72-83	4.7	46
35	Bioinformatic methods in NMR-based metabolic profiling. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2009**, 55, 361-374	10.4	82
34	Statistical total correlation spectroscopy editing of 1H NMR spectra of biofluids: application to drug metabolite profile identification and enhanced information recovery. *Analytical Chemistry*, **2009**, 81, 6458-66	7.8	37
33	Analytic properties of statistical total correlation spectroscopy based information recovery in 1H NMR metabolic data sets. *Analytical Chemistry*, **2009**, 81, 2075-84	7.8	51
32	Cluster analysis statistical spectroscopy using nuclear magnetic resonance generated metabolic data sets from perturbed biological systems. *Analytical Chemistry*, **2009**, 81, 6581-9	7.8	30
31	Metabolic profiling and population screening of analgesic usage in nuclear magnetic resonance spectroscopy-based large-scale epidemiologic studies. *Analytical Chemistry*, **2009**, 81, 5119-29	7.8	36
30	Recursive segment-wise peak alignment of biological (1)h NMR spectra for improved metabolic biomarker recovery. *Analytical Chemistry*, **2009**, 81, 56-66	7.8	258
29	Human metabolic phenotype diversity and its association with diet and blood pressure. *Nature*, **2008**, 453, 396-400	50.4	847
28	Piecewise multivariate modelling of sequential metabolic profiling data. *BMC Bioinformatics*, **2008**, 9, 105	3.6	23

27	Temporal metabonomic modeling of l-arginine-induced exocrine pancreatitis. *Journal of Proteome Research*, **2008**, 7, 4435-45	5.6	49
26	The carcinoGENOMICS project: critical selection of model compounds for the development of omics-based in vitro carcinogenicity screening assays. *Mutation Research - Reviews in Mutation Research*, **2008**, 659, 202-10	7	50
25	Statistical Techniques in Metabolic Profiling **2008**, 347-373		9
24	Robust algorithms for automated chemical shift calibration of 1D 1H NMR spectra of blood serum. *Analytical Chemistry*, **2008**, 80, 7158-62	7.8	52
23	Metabolic profiling, metabolomic and metabonomic procedures for NMR spectroscopy of urine, plasma, serum and tissue extracts. *Nature Protocols*, **2007**, 2, 2692-703	18.8	1536
22	Proposed minimum reporting standards for data analysis in metabolomics. *Metabolomics*, **2007**, 3, 231-241	4.7	317
21	Non-linear Methods for the Analysis of Metabolic Profiles **2007**, 201-226		3
20	Prediction and classification of drug toxicity using probabilistic modeling of temporal metabolic data: the consortium on metabonomic toxicology screening approach. *Journal of Proteome Research*, **2007**, 6, 4407-22	5.6	146
19	springScape: visualisation of microarray and contextual bioinformatic data using spring embedding and an 'information landscape'. *Bioinformatics*, **2006**, 22, e99-107	7.2	16
18	Comparative metabonomics of differential hydrazine toxicity in the rat and mouse. *Toxicology and Applied Pharmacology*, **2005**, 204, 135-51	4.6	107
17	The Consortium for Metabonomic Toxicology (COMET): aims, activities and achievements. *Pharmacogenomics*, **2005**, 6, 691-9	2.6	255
16	Evaluation of metabolic variation in normal rat strains from a statistical analysis of 1H NMR spectra of urine. *Journal of Pharmaceutical and Biomedical Analysis*, **2004**, 36, 823-33	3.5	32
15	Statistical experimental design and partial least squares regression analysis of biofluid metabonomic NMR and clinical chemistry data for screening of adverse drug effects. *Chemometrics and Intelligent Laboratory Systems*, **2004**, 73, 139-149	3.8	57
14	Geometric trajectory analysis of metabolic responses to toxicity can define treatment specific profiles. *Chemical Research in Toxicology*, **2004**, 17, 579-87	4	131
13	Spectral editing and pattern recognition methods applied to high-resolution magic-angle spinning 1H nuclear magnetic resonance spectroscopy of liver tissues. *Analytical Biochemistry*, **2003**, 323, 26-32	3.1	134
12	Contemporary issues in toxicology the role of metabonomics in toxicology and its evaluation by the COMET project. *Toxicology and Applied Pharmacology*, **2003**, 187, 137-46	4.6	342
11	NMR-based metabonomic toxicity classification: hierarchical cluster analysis and k-nearest-neighbour approaches. *Analytica Chimica Acta*, **2003**, 490, 3-15	6.6	127
10	Improved analysis of multivariate data by variable stability scaling: application to NMR-based metabolic profiling. *Analytica Chimica Acta*, **2003**, 490, 265-276	6.6	149

9	Toxicity classification from metabonomic data using a density superposition approach: CLOUDS. *Analytica Chimica Acta*, **2003**, 490, 109-122	6.6	69
8	Semiempirical Molecular-Orbital Properties of Some Polycyclic Aromatic Hydrocarbons and Correlation with Environmental Toxic Equivalency Factors. *Polycyclic Aromatic Compounds*, **2003**, 23, 23-47	1.3	2
7	Batch statistical processing of 1H NMR-derived urinary spectral data. *Journal of Chemometrics*, **2002**, 16, 461-468	1.6	80
6	Analytical reproducibility in (1)H NMR-based metabonomic urinalysis. *Chemical Research in Toxicology*, **2002**, 15, 1380-6	4	239
5	Quantitative Investigation of Probabilistic Spectral Processing Methods Using Simulated NMR Data. *Applied Spectroscopy*, **2001**, 55, 1214-1224	3.1	6
4	Spectroscopic confirmation of redshifts predicted by gravitational lensing. *Monthly Notices of the Royal Astronomical Society*, **1998**, 295, 75	4.3	16
3	Identification of a gravitationally lensed z = 2.515 star-forming galaxy. *Monthly Notices of the Royal Astronomical Society*, **1996**, 281, L75-L81	4.3	45
2	PhenoMeNal: Processing and analysis of Metabolomics data in the Cloud		1
1	Estimation of permutation-based metabolome-wide significance thresholds		1