

# Timothy Ebbels

## List of Publications by Year in descending order

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143  
papers

11,538  
citations

41627

51  
h-index

33145

104  
g-index

151  
all docs

151  
docs citations

151  
times ranked

15322  
citing authors

| #  | ARTICLE   | IF  | CITATIONS |
|----|---|-----|-----------|
| 1  | Automated Annotation of Untargeted All-Ion Fragmentation LC-MS Metabolomics Data with MetaboAnnotator. <i>Analytical Chemistry</i> , 2022, 94, 3446-3455.   | 3.2 | 18        |
| 2  | Finding Correspondence between Metabolomic Features in Untargeted Liquid Chromatography-Mass Spectrometry Metabolomics Datasets. <i>Analytical Chemistry</i> , 2022, 94, 5493-5503.   | 3.2 | 9         |
| 3  | Blood pressure interactions with the DASH dietary pattern, sodium, and potassium: The International Study of Macro-/Micronutrients and Blood Pressure (INTERMAP). <i>American Journal of Clinical Nutrition</i> , 2022, 116, 216-229.                 | 2.2 | 13        |
| 4  | Metabolomics: The Stethoscope for the Twenty-First Century. <i>Medical Principles and Practice</i> , 2021, 30, 301-310.   | 1.1 | 46        |
| 5  | Multiple-testing correction in metabolome-wide association studies. <i>BMC Bioinformatics</i> , 2021, 22, 67.   | 1.2 | 13        |
| 6  | Bayesian Deconvolution and Quantification of Metabolites from J-Resolved NMR Spectroscopy. <i>Bayesian Analysis</i> , 2021, 16, .   | 1.6 | 3         |
| 7  | Statistical analysis in metabolic phenotyping. <i>Nature Protocols</i> , 2021, 16, 4299-4326.   | 5.5 | 40        |
| 8  | Pathway analysis in metabolomics: Recommendations for the use of over-representation analysis. <i>PLoS Computational Biology</i> , 2021, 17, e1009105.  | 1.5 | 59        |
| 9  | Progress towards an OECD reporting framework for transcriptomics and metabolomics in regulatory toxicology. <i>Regulatory Toxicology and Pharmacology</i> , 2021, 125, 105020.  | 1.3 | 46        |
| 10 | The association of fish consumption and its urinary metabolites with cardiovascular risk factors: the International Study of Macro-/Micronutrients and Blood Pressure (INTERMAP). <i>American Journal of Clinical Nutrition</i> , 2020, 111, 280-290. | 2.2 | 37        |
| 11 | Metabolic Signatures of Gestational Weight Gain and Postpartum Weight Loss in a Lifestyle Intervention Study of Overweight and Obese Women. <i>Metabolites</i> , 2020, 10, 498.   | 1.3 | 5         |
| 12 | Extraction and Integration of Genetic Networks from Short-Profile Omic Data Sets. <i>Metabolites</i> , 2020, 10, 435.   | 1.3 | 6         |
| 13 | Targeted realignment of LC-MS profiles by neighbor-wise compound-specific graphical time warping with misalignment detection. <i>Bioinformatics</i> , 2020, 36, 2862-2871.  | 1.8 | 14        |
| 14 | Integrative analysis of time course metabolic data and biomarker discovery. <i>BMC Bioinformatics</i> , 2020, 21, 11.   | 1.2 | 11        |
| 15 | Abstract MP45: A Metabolome-wide Association Study of Plant Food Consumption With Blood Pressure. <i>Circulation</i> , 2020, 141, .   | 1.6 | 0         |
| 16 | Data mining and visualisation: general discussion. <i>Faraday Discussions</i> , 2019, 218, 354-371.   | 1.6 | 2         |
| 17 | Use cases, best practice and reporting standards for metabolomics in regulatory toxicology. <i>Nature Communications</i> , 2019, 10, 3041.  | 5.8 | 131       |
| 18 | Predictive modelling using pathway scores: robustness and significance of pathway collections. <i>BMC Bioinformatics</i> , 2019, 20, 543.   | 1.2 | 17        |

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|----|---|-----|-----------|
| 19 | Comparison of Bi- and Tri-Linear PLS Models for Variable Selection in Metabolomic Time-Series Experiments. <i>Metabolites</i> , 2019, 9, 92.  | 1.3 | 3         |
| 20 | Serum metabolic signatures of coronary and carotid atherosclerosis and subsequent cardiovascular disease. <i>European Heart Journal</i> , 2019, 40, 2883-2896.  | 1.0 | 107       |
| 21 | PhenoMeNal: processing and analysis of metabolomics data in the cloud. <i>GigaScience</i> , 2019, 8, .  | 3.3 | 60        |
| 22 | Big Data and Databases for Metabolic Phenotyping. , 2019, , 329-367.  |     | 2         |
| 23 | Processing and Analysis of Untargeted Multicohort NMR Data. <i>Methods in Molecular Biology</i> , 2019, 2037, 453-470.  | 0.4 | 2         |
| 24 | Abstract P228: Relationships of Dietary and Supplement Magnesium Intake and Its Urinary Metabolomic Biomarkers With Blood Pressure: The INTERMAP Study. <i>Circulation</i> , 2019, 139, .   | 1.6 | 0         |
| 25 | Abstract P229: Cross-Sectional Investigation of the Relationship Between Fish Consumption and Its Urinary Biomarkers With Blood Pressure Across Asian and Western Populations: Results From the INTERMAP Study. <i>Circulation</i> , 2019, 139, . | 1.6 | 0         |
| 26 | Optimized Phenotypic Biomarker Discovery and Confounder Elimination via Covariate-Adjusted Projection to Latent Structures from Metabolic Spectroscopy Data. <i>Journal of Proteome Research</i> , 2018, 17, 1586-1595.                           | 1.8 | 29        |
| 27 | A comparison of human serum and plasma metabolites using untargeted 1H NMR spectroscopy and UPLC-MS. <i>Metabolomics</i> , 2018, 14, 32.  | 1.4 | 31        |
| 28 | nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. <i>Analytical Chemistry</i> , 2018, 90, 649-656.  | 3.2 | 50        |
| 29 | MEtabolomics standaRds Initiative in Toxicology (MERIT). <i>Toxicology Letters</i> , 2018, 295, S214.   | 0.4 | 2         |
| 30 | Bayesian estimation of the number of protonation sites for urinary metabolites from NMR spectroscopic data. <i>Metabolomics</i> , 2018, 14, 56.   | 1.4 | 13        |
| 31 | Reliability of plasma polar metabolite concentrations in a large-scale cohort study using capillary electrophoresis-mass spectrometry. <i>PLoS ONE</i> , 2018, 13, e0191230.  | 1.1 | 58        |
| 32 | Advances in Computational Analysis of Metabolomic NMR Data. <i>New Developments in NMR</i> , 2018, , 310-323.   | 0.1 | 1         |
| 33 | Computational tools and workflows in metabolomics: An international survey highlights the opportunity for harmonisation through Galaxy. <i>Metabolomics</i> , 2017, 13, 12.   | 1.4 | 69        |
| 34 | Metabolic phenotyping for discovery of urinary biomarkers of diet, xenobiotics and blood pressure in the INTERMAP Study: an overview. <i>Hypertension Research</i> , 2017, 40, 336-345.   | 1.5 | 14        |
| 35 | Applying 'omics technologies in chemicals risk assessment: Report of an ECETOC workshop. <i>Regulatory Toxicology and Pharmacology</i> , 2017, 91, S3-S13.  | 1.3 | 102       |
| 36 | Framework for the quality assurance of 'omics technologies considering GLP requirements. <i>Regulatory Toxicology and Pharmacology</i> , 2017, 91, S27-S35.   | 1.3 | 32        |

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|----|---|-----|-----------|
| 37 | Improving Visualization and Interpretation of Metabolome-Wide Association Studies: An Application in a Population-Based Cohort Using Untargeted <sup>1</sup> H NMR Metabolic Profiling. Journal of Proteome Research, 2017, 16, 3623-3633.  | 1.8 | 26        |
| 38 | Bayesian inference for multiple Gaussian graphical models with application to metabolic association networks. Annals of Applied Statistics, 2017, 11, .   | 0.5 | 23        |
| 39 | The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.   | 0.8 | 19        |
| 40 | The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.   | 0.8 | 11        |
| 41 | Synergistic and Antagonistic Mutation Responses of Human MCL-5 Cells to Mixtures of Benzo[ <i>a</i> ]pyrene and 2-Amino-1-Methyl-6-Phenylimidazo[4,5- <i>b</i> ]pyridine: Dose-Related Variation in the Joint Effects of Common Dietary Carcinogens. Environmental Health Perspectives, 2016, 124, 88-96. | 2.8 | 21        |
| 42 | Urinary hippurate and proline betaine relative to fruit intake, blood pressure, and body mass index. Proceedings of the Nutrition Society, 2016, 75, .  | 0.4 | 1         |
| 43 | Power Analysis and Sample Size Determination in Metabolic Phenotyping. Analytical Chemistry, 2016, 88, 5179-5188.   | 3.2 | 95        |
| 44 | Modelling the acid/base <sup>1</sup> H NMR chemical shift limits of metabolites in human urine. Metabolomics, 2016, 12, 152.  | 1.4 | 47        |
| 45 | Workflow for Integrated Processing of Multicohort Untargeted <sup>1</sup> H NMR Metabolomics Data in Large-Scale Metabolic Epidemiology. Journal of Proteome Research, 2016, 15, 4188-4194.   | 1.8 | 37        |
| 46 | Data standards can boost metabolomics research, and if there is a will, there is a way. Metabolomics, 2016, 12, 14.   | 1.4 | 97        |
| 47 | Statistical Correlations between NMR Spectroscopy and Direct Infusion FT-ICR Mass Spectrometry Aid Annotation of Unknowns in Metabolomics. Analytical Chemistry, 2016, 88, 2583-2589.   | 3.2 | 25        |
| 48 | One minute with the Metabolomics Society's Honorary Fellows 2015. Metabolomics, 2015, 11, 779-781.  | 1.4 | 0         |
| 49 | COordination of Standards in MetabOmicS (COSMOS): facilitating integrated metabolomics data access. Metabolomics, 2015, 11, 1587-1597.  | 1.4 | 140       |
| 50 | diXa: a data infrastructure for chemical safety assessment. Bioinformatics, 2015, 31, 1505-1507.  | 1.8 | 40        |
| 51 | The international Metabolomics Society in 2015: the path forward to success. Metabolomics, 2015, 11, 1-2.   | 1.4 | 7         |
| 52 | Over-representation of correlation analysis (ORCA): a method for identifying associations between variable sets. Bioinformatics, 2015, 31, 102-108.   | 1.8 | 9         |
| 53 | Urinary metabolic signatures of human adiposity. Science Translational Medicine, 2015, 7, 285ra62.  | 5.8 | 178       |
| 54 | Ask not what your Society can do for you, ask what you can do for your Society!. Metabolomics, 2015, 11, 499-500.   | 1.4 | 0         |

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|----|---|-----|-----------|
| 55 | Results of the 2015 elections to the board of directors. <i>Metabolomics</i> , 2015, 11, 1473-1474.   | 1.4 | 0         |
| 56 | Embedding standards in metabolomics: the Metabolomics Society data standards task group. <i>Metabolomics</i> , 2015, 11, 782-783.   | 1.4 | 13        |
| 57 | Orders of Magnitude Extension of the Effective Dynamic Range of TDC-Based TOFMS Data Through Maximum Likelihood Estimation. <i>Journal of the American Society for Mass Spectrometry</i> , 2014, 25, 1824-1827.   | 1.2 | 4         |
| 58 | Variance and covariance heterogeneity analysis for detection of metabolites associated with cadmium exposure. <i>Statistical Applications in Genetics and Molecular Biology</i> , 2014, 13, 191-201.  | 0.2 | 4         |
| 59 | Identifying biochemical phenotypic differences between cryptic species. <i>Biology Letters</i> , 2014, 10, 20140615.  | 1.0 | 13        |
| 60 | Bayesian deconvolution and quantification of metabolites in complex 1D NMR spectra using BATMAN. <i>Nature Protocols</i> , 2014, 9, 1416-1427.  | 5.5 | 167       |
| 61 | Design and Analysis of Metabolomics Studies in Epidemiologic Research: A Primer on -Omic Technologies. <i>American Journal of Epidemiology</i> , 2014, 180, 129-139.  | 1.6 | 152       |
| 62 | Genome metabolome integrated network analysis to uncover connections between genetic variants and complex traits: an application to obesity. <i>Journal of the Royal Society Interface</i> , 2014, 11, 20130908.  | 1.5 | 20        |
| 63 | <sup>1</sup> H NMR-Based Profiling Reveals Differential Immune-Metabolic Networks during Influenza Virus Infection in Obese Mice. <i>PLoS ONE</i> , 2014, 9, e97238.  | 1.1 | 25        |
| 64 | Proteomic and metabolomic responses to connexin43 silencing in primary hepatocyte cultures. <i>Archives of Toxicology</i> , 2013, 87, 883-894.  | 1.9 | 12        |
| 65 | The continuing growth and development of YOUR metabolomics society. <i>Metabolomics</i> , 2013, 9, 529-531.   | 1.4 | 0         |
| 66 | Report on the 9th Annual International Conference of the Metabolomics Society. <i>Metabolomics</i> , 2013, 9, 935-937.  | 1.4 | 0         |
| 67 | A Combination of Transcriptomics and Metabolomics Uncovers Enhanced Bile Acid Biosynthesis in HepG2 Cells Expressing CCAAT/Enhancer-Binding Protein $\beta$ (C/EBP $\beta$ ), Hepatocyte Nuclear Factor 4 $\alpha$ (HNF4 $\alpha$ ), and Constitutive Androstane Receptor (CAR). <i>Journal of Proteome Research</i> , 2013, 12, 2732-2741. | 1.8 | 5         |
| 68 | Combining Spectral Ordering with Peak Fitting for One-Dimensional NMR Quantitative Metabolomics. <i>Analytical Chemistry</i> , 2013, 85, 4605-4612.   | 3.2 | 19        |
| 69 | Integrated Histopathological and Urinary Metabonomic Investigation of the Pathogenesis of Microcystin-LR Toxicosis. <i>Veterinary Pathology</i> , 2013, 50, 159-171.  | 0.8 | 16        |
| 70 | Dietary and Urinary Metabonomic Factors Possibly Accounting for Higher Blood Pressure of Black Compared With White Americans. <i>Hypertension</i> , 2013, 62, 1074-1080.  | 1.3 | 24        |
| 71 | Untargeted Metabolome Quantitative Trait Locus Mapping Associates Variation in Urine Glycerate to Mutant Glycerate Kinase. <i>Journal of Proteome Research</i> , 2012, 11, 631-642.   | 1.8 | 25        |
| 72 | BATMAN <sup>®</sup> an R package for the automated quantification of metabolites from nuclear magnetic resonance spectra using a Bayesian model. <i>Bioinformatics</i> , 2012, 28, 2088-2090.   | 1.8 | 142       |

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|----|--|-----|-----------|
| 73 | A Bayesian Model of NMR Spectra for the Deconvolution and Quantification of Metabolites in Complex Biological Mixtures. <i>Journal of the American Statistical Association</i> , 2012, 107, 1259-1271.   | 1.8 | 41        |
| 74 | Intra- and Interlaboratory Reproducibility of Ultra Performance Liquid Chromatographyâ€“Time-of-Flight Mass Spectrometry for Urinary Metabolic Profiling. <i>Analytical Chemistry</i> , 2012, 84, 2424-2432.                                       | 3.2 | 44        |
| 75 | Subset Optimization by Reference Matching (STORM): An Optimized Statistical Approach for Recovery of Metabolic Biomarker Structural Information from <sup>1</sup> H NMR Spectra of Biofluids. <i>Analytical Chemistry</i> , 2012, 84, 10694-10701. | 3.2 | 75        |
| 76 | Optimizing the Use of Quality Control Samples for Signal Drift Correction in Large-Scale Urine Metabolic Profiling Studies. <i>Analytical Chemistry</i> , 2012, 84, 2670-2677.   | 3.2 | 127       |
| 77 | Characterization of data analysis methods for information recovery from metabolic <sup>1</sup> H NMR spectra using artificial complex mixtures. <i>Metabolomics</i> , 2012, 8, 1170-1180.  | 1.4 | 3         |
| 78 | Prospects for a Statistical Theory of LC/TOFMS Data. <i>Journal of the American Society for Mass Spectrometry</i> , 2012, 23, 779-791.   | 1.2 | 8         |
| 79 | Metabolic response to low-level toxicant exposure in a novel renal tubuleepithelial cell system. <i>Molecular BioSystems</i> , 2011, 7, 247-257.   | 2.9 | 60        |
| 80 | Response to Comment on â€œOptimized Preprocessing of Ultra-Performance Liquid Chromatography/Mass Spectrometry Urinary Metabolic Profiles for Improved Information Recoveryâ€. <i>Analytical Chemistry</i> , 2011, 83, 9721-9722.                 | 3.2 | 2         |
| 81 | Optimized Preprocessing of Ultra-Performance Liquid Chromatography/Mass Spectrometry Urinary Metabolic Profiles for Improved Information Recovery. <i>Analytical Chemistry</i> , 2011, 83, 5864-5872.  | 3.2 | 240       |
| 82 | Data-Driven Approach for Metabolite Relationship Recovery in Biological <sup>1</sup> H NMR Data Sets Using Iterative Statistical Total Correlation Spectroscopy. <i>Analytical Chemistry</i> , 2011, 83, 2075-2082.                                | 3.2 | 52        |
| 83 | A statistical framework for biomarker discovery in metabolomic time course data. <i>Bioinformatics</i> , 2011, 27, 1979-1985.  | 1.8 | 41        |
| 84 | Modelling Short Time Series in Metabolomics: A Functional Data Analysis Approach. <i>Advances in Experimental Medicine and Biology</i> , 2011, 696, 307-315.   | 0.8 | 12        |
| 85 | Meeting-in-the-middle using metabolic profiling â€“ a strategy for the identification of intermediate biomarkers in cohort studies. <i>Biomarkers</i> , 2011, 16, 83-88.   | 0.9 | 113       |
| 86 | Consensus-Phenotype Integration of Transcriptomic and Metabolomic Data Implies a Role for Metabolism in the Chemosensitivity of Tumour Cells. <i>PLoS Computational Biology</i> , 2011, 7, e1001113.   | 1.5 | 83        |
| 87 | Integrated pathway-level analysis of transcriptomics and metabolomics data with IMPaLA. <i>Bioinformatics</i> , 2011, 27, 2917-2918.   | 1.8 | 356       |
| 88 | Processing and Modeling of Nuclear Magnetic Resonance (NMR) Metabolic Profiles. <i>Methods in Molecular Biology</i> , 2011, 708, 365-388.  | 0.4 | 25        |
| 89 | A Differential Network Approach to Exploring Differences between Biological States: An Application to Prediabetes. <i>PLoS ONE</i> , 2011, 6, e24702.  | 1.1 | 33        |
| 90 | Metabolic Profiling and the Metabolome-Wide Association Study: Significance Level For Biomarker Identification. <i>Journal of Proteome Research</i> , 2010, 9, 4620-4627.  | 1.8 | 123       |

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|-----|---|-----|-----------|
| 91  | MetAssimulo:Simulation of Realistic NMR Metabolic Profiles. BMC Bioinformatics, 2010, 11, 496.  | 1.2 | 17        |
| 92  | The evolution of partial least squares models and related chemometric approaches in metabonomics and metabolic phenotyping. Journal of Chemometrics, 2010, 24, 636-649.   | 0.7 | 140       |
| 93  | Intra- and inter-omic fusion of metabolic profiling data in a systems biology framework. Chemometrics and Intelligent Laboratory Systems, 2010, 104, 121-131.   | 1.8 | 51        |
| 94  | 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. | 3.0 | 52        |
| 95  | High-resolution magic-angle-spinning NMR spectroscopy for metabolic profiling of intact tissues. Nature Protocols, 2010, 5, 1019-1032.  | 5.5 | 355       |
| 96  | 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, 6647-6654.  | 1.8 | 116       |
| 97  | Bidirectional Correlation of NMR and Capillary Electrophoresis Fingerprints: A New Approach to Investigating <i>Schistosoma mansoni</i> Infection in a Mouse Model. Analytical Chemistry, 2010, 82, 203-210.                            | 3.2 | 28        |
| 98  | A Statistically Rigorous Test for the Identification of Parent-Fragment Pairs in LC-MS Datasets. Analytical Chemistry, 2010, 82, 1766-1778.   | 3.2 | 26        |
| 99  | Effect of the Histone Deacetylase Inhibitor Trichostatin A on the Metabolome of Cultured Primary Hepatocytes. Journal of Proteome Research, 2010, 9, 413-419.   | 1.8 | 12        |
| 100 | Construction of Confidence Regions for Isotopic Abundance Patterns in LC/MS Data Sets for Rigorous Determination of Molecular Formulas. Analytical Chemistry, 2010, 82, 7319-7328.  | 3.2 | 10        |
| 101 | NMR-Based Metabolic Profiling Identifies Biomarkers of Liver Regeneration Following Partial Hepatectomy in the Rat. Journal of Proteome Research, 2010, 9, 59-69.   | 1.8 | 75        |
| 102 | A Combined Metabonomic and Transcriptomic Approach to Investigate Metabolism during Development in the Chick Chorioallantoic Membrane. Journal of Proteome Research, 2010, 9, 3126-3134.  | 1.8 | 15        |
| 103 | Opening up the "Black Box": Metabolic phenotyping and metabolome-wide association studies in epidemiology. Journal of Clinical Epidemiology, 2010, 63, 970-979.   | 2.4 | 125       |
| 104 | Optimization and Evaluation of Metabolite Extraction Protocols for Untargeted Metabolic Profiling of Liver Samples by UPLC-MS. Analytical Chemistry, 2010, 82, 7779-7786.   | 3.2 | 160       |
| 105 | Correction of mass calibration gaps in liquid chromatography-mass spectrometry metabolomics data. Bioinformatics, 2010, 26, 2488-2489.  | 1.8 | 195       |
| 106 | Genetic algorithms for simultaneous variable and sample selection in metabonomics. Bioinformatics, 2009, 25, 112-118.   | 1.8 | 56        |
| 107 | Time-Resolved Metabolic Footprinting for Nonlinear Modeling of Bacterial Substrate Utilization. Applied and Environmental Microbiology, 2009, 75, 2453-2463.  | 1.4 | 52        |
| 108 | Metabonomic investigations into the global biochemical sequelae of exposure to the pancreatic toxin 1-cyano-2-acetyl-3-butene in the rat. Magnetic Resonance in Chemistry, 2009, 47, S26-35.  | 1.1 | 14        |

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|-----|--|------|-----------|
| 109 | Validation of metabolomics for toxic mechanism of action screening with the earthworm <i>Lumbricus rubellus</i> . <i>Metabolomics</i> , 2009, 5, 72-83.  | 1.4  | 48        |
| 110 | Bioinformatic methods in NMR-based metabolic profiling. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2009, 55, 361-374.  | 3.9  | 91        |
| 111 | Statistical Total Correlation Spectroscopy Editing of <sup>1</sup> H NMR Spectra of Biofluids: Application to Drug Metabolite Profile Identification and Enhanced Information Recovery. <i>Analytical Chemistry</i> , 2009, 81, 6458-6466. | 3.2  | 38        |
| 112 | Analytic Properties of Statistical Total Correlation Spectroscopy Based Information Recovery in <sup>1</sup> H NMR Metabolic Data Sets. <i>Analytical Chemistry</i> , 2009, 81, 2075-2084.   | 3.2  | 56        |
| 113 | Cluster Analysis Statistical Spectroscopy Using Nuclear Magnetic Resonance Generated Metabolic Data Sets from Perturbed Biological Systems. <i>Analytical Chemistry</i> , 2009, 81, 6581-6589.   | 3.2  | 36        |
| 114 | Metabolic Profiling and Population Screening of Analgesic Usage in Nuclear Magnetic Resonance Spectroscopy-Based Large-Scale Epidemiologic Studies. <i>Analytical Chemistry</i> , 2009, 81, 5119-5129.                                     | 3.2  | 37        |
| 115 | Recursive Segment-Wise Peak Alignment of Biological <sup>1</sup> H NMR Spectra for Improved Metabolic Biomarker Recovery. <i>Analytical Chemistry</i> , 2009, 81, 56-66.   | 3.2  | 303       |
| 116 | Statistical Techniques in Metabolic Profiling. , 2008, , 347-373.  |      | 13        |
| 117 | Robust Algorithms for Automated Chemical Shift Calibration of 1D <sup>1</sup> H NMR Spectra of Blood Serum. <i>Analytical Chemistry</i> , 2008, 80, 7158-7162.   | 3.2  | 58        |
| 118 | Human metabolic phenotype diversity and its association with diet and blood pressure. <i>Nature</i> , 2008, 453, 396-400.  | 13.7 | 966       |
| 119 | Piecewise multivariate modelling of sequential metabolic profiling data. <i>BMC Bioinformatics</i> , 2008, 9, 105.   | 1.2  | 24        |
| 120 | Temporal Metabonomic Modeling of <sup>1</sup> Arginine-Induced Exocrine Pancreatitis. <i>Journal of Proteome Research</i> , 2008, 7, 4435-4445.  | 1.8  | 55        |
| 121 | The carcinoGENOMICS project: Critical selection of model compounds for the development of omics-based in vitro carcinogenicity screening assays. <i>Mutation Research - Reviews in Mutation Research</i> , 2008, 659, 202-210.             | 2.4  | 60        |
| 122 | Non-linear Methods for the Analysis of Metabolic Profiles. , 2007, , 201-226.  |      | 7         |
| 123 | Prediction and Classification of Drug Toxicity Using Probabilistic Modeling of Temporal Metabolic Data: The Consortium on Metabonomic Toxicology Screening Approach. <i>Journal of Proteome Research</i> , 2007, 6, 4407-4422.             | 1.8  | 164       |
| 124 | Metabolic profiling, metabolomic and metabonomic procedures for NMR spectroscopy of urine, plasma, serum and tissue extracts. <i>Nature Protocols</i> , 2007, 2, 2692-2703.  | 5.5  | 1,830     |
| 125 | Proposed minimum reporting standards for data analysis in metabolomics. <i>Metabolomics</i> , 2007, 3, 231-241.  | 1.4  | 361       |
| 126 | springScape: visualisation of microarray and contextual bioinformatic data using spring embedding and an 'information landscape'. <i>Bioinformatics</i> , 2006, 22, e99-e107.  | 1.8  | 22        |



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|-----|--|-----|-----------|
| 127 | We-P14:381 Metabonomics to assess self-reported data: The international study on macronutrients and blood pressure (INTERMAP). <i>Atherosclerosis Supplements</i> , 2006, 7, 430-431.  | 1.2 | 0         |
| 128 | Comparative metabonomics of differential hydrazine toxicity in the rat and mouse. <i>Toxicology and Applied Pharmacology</i> , 2005, 204, 135-151.   | 1.3 | 125       |
| 129 | The Consortium for Metabonomic Toxicology (COMET): aims, activities and achievements. <i>Pharmacogenomics</i> , 2005, 6, 691-699.  | 0.6 | 277       |
| 130 | Evaluation of metabolic variation in normal rat strains from a statistical analysis of <sup>1</sup> H NMR spectra of urine. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2004, 36, 823-833.  | 1.4 | 33        |
| 131 | Statistical experimental design and partial least squares regression analysis of biofluid metabonomic NMR and clinical chemistry data for screening of adverse drug effects. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2004, 73, 139-149. | 1.8 | 64        |
| 132 | Geometric Trajectory Analysis of Metabolic Responses To Toxicity Can Define Treatment Specific Profiles. <i>Chemical Research in Toxicology</i> , 2004, 17, 579-587.   | 1.7 | 143       |
| 133 | Spectral editing and pattern recognition methods applied to high-resolution magic-angle spinning <sup>1</sup> H nuclear magnetic resonance spectroscopy of liver tissues. <i>Analytical Biochemistry</i> , 2003, 323, 26-32.                             | 1.1 | 144       |
| 134 | Contemporary issues in toxicology the role of metabonomics in toxicology and its evaluation by the COMET project. <i>Toxicology and Applied Pharmacology</i> , 2003, 187, 137-146.   | 1.3 | 374       |
| 135 | NMR-based metabonomic toxicity classification: hierarchical cluster analysis and k-nearest-neighbour approaches. <i>Analytica Chimica Acta</i> , 2003, 490, 3-15.  | 2.6 | 142       |
| 136 | Improved analysis of multivariate data by variable stability scaling: application to NMR-based metabolic profiling. <i>Analytica Chimica Acta</i> , 2003, 490, 265-276.  | 2.6 | 164       |
| 137 | Toxicity classification from metabonomic data using a density superposition approach: "CLOUDS"™. <i>Analytica Chimica Acta</i> , 2003, 490, 109-122.   | 2.6 | 76        |
| 138 | Semiempirical Molecular-Orbital Properties of Some Polycyclic Aromatic Hydrocarbons and Correlation with Environmental Toxic Equivalency Factors. <i>Polycyclic Aromatic Compounds</i> , 2003, 23, 23-47.  | 1.4 | 2         |
| 139 | Batch statistical processing of <sup>1</sup> H NMR-derived urinary spectral data. <i>Journal of Chemometrics</i> , 2002, 16, 461-468.  | 0.7 | 82        |
| 140 | Analytical Reproducibility in <sup>1</sup> H NMR-Based Metabonomic Urinalysis. <i>Chemical Research in Toxicology</i> , 2002, 15, 1380-1386.   | 1.7 | 261       |
| 141 | Quantitative Investigation of Probabilistic Spectral Processing Methods Using Simulated NMR Data. <i>Applied Spectroscopy</i> , 2001, 55, 1214-1224.   | 1.2 | 6         |
| 142 | Spectroscopic confirmation of redshifts predicted by gravitational lensing. <i>Monthly Notices of the Royal Astronomical Society</i> , 1998, 295, 75.  | 1.6 | 19        |
| 143 | Identification of a gravitationally lensed z = 2.515 star-forming galaxy. <i>Monthly Notices of the Royal Astronomical Society</i> , 1996, 281, L75-L81.   | 1.6 | 47        |