

# Jeremy K Nicholson

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/6282995/publications.pdf>

Version: 2024-02-01

791  
papers

91,144  
citations

299

139  
h-index

507

268  
g-index

828  
all docs

828  
docs citations

828  
times ranked

59662  
citing authors

#	ARTICLE	IF	CITATIONS
1	Host-Gut Microbiota Metabolic Interactions. <i>Science</i> , 2012, 336, 1262-1267.	12.6	3,693
2	'Metabonomics': understanding the metabolic responses of living systems to pathophysiological stimuli via multivariate statistical analysis of biological NMR spectroscopic data. <i>Xenobiotica</i> , 1999, 29, 1181-1189.	1.1	3,429
3	Metabolic profiling, metabolomic and metabonomic procedures for NMR spectroscopy of urine, plasma, serum and tissue extracts. <i>Nature Protocols</i> , 2007, 2, 2692-2703.	12.0	1,830
4	Metabonomics: a platform for studying drug toxicity and gene function. <i>Nature Reviews Drug Discovery</i> , 2002, 1, 153-161.	46.4	1,739
5	Metabonomics. <i>Nature</i> , 2008, 455, 1054-1056.	27.8	1,660
6	OPLS discriminant analysis: combining the strengths of PLS-DA and SIMCA classification. <i>Journal of Chemometrics</i> , 2006, 20, 341-351.	1.3	1,134
7	Gut Microbiomes of Malawian Twin Pairs Discordant for Kwashiorkor. <i>Science</i> , 2013, 339, 548-554.	12.6	1,012
8	Impact of the gut microbiota on inflammation, obesity, and metabolic disease. <i>Genome Medicine</i> , 2016, 8, 42.	8.2	1,000
9	Symbiotic gut microbes modulate human metabolic phenotypes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 2117-2122.	7.1	994
10	Understanding 'Global' Systems Biology: Metabonomics and the Continuum of Metabolism. <i>Nature Reviews Drug Discovery</i> , 2003, 2, 668-676.	46.4	975
11	750 MHz <sup>1</sup> H and <sup>1</sup> H- <sup>13</sup> C NMR Spectroscopy of Human Blood Plasma. <i>Analytical Chemistry</i> , 1995, 67, 793-811.	6.5	972
12	Human metabolic phenotype diversity and its association with diet and blood pressure. <i>Nature</i> , 2008, 453, 396-400.	27.8	966
13	Metabolic profiling reveals a contribution of gut microbiota to fatty liver phenotype in insulin-resistant mice. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 12511-12516.	7.1	948
14	Rapid and noninvasive diagnosis of the presence and severity of coronary heart disease using <sup>1</sup> H-NMR-based metabonomics. <i>Nature Medicine</i> , 2002, 8, 1439-1445.	30.7	941
15	Global metabolic profiling procedures for urine using UPLC-MS. <i>Nature Protocols</i> , 2010, 5, 1005-1018.	12.0	867
16	Gut microorganisms, mammalian metabolism and personalized health care. <i>Nature Reviews Microbiology</i> , 2005, 3, 431-438.	28.6	861
17	Statistical Total Correlation Spectroscopy: An Exploratory Approach for Latent Biomarker Identification from Metabolic <sup>1</sup> H NMR Data Sets. <i>Analytical Chemistry</i> , 2005, 77, 1282-1289.	6.5	833
18	Pharmaco-metabonomic phenotyping and personalized drug treatment. <i>Nature</i> , 2006, 440, 1073-1077.	27.8	787

#	ARTICLE	IF	CITATIONS
19	Global metabolic profiling of animal and human tissues via UPLC-MS. <i>Nature Protocols</i> , 2013, 8, 17-32.	12.0	774
20	Fat, fibre and cancer risk in African Americans and rural Africans. <i>Nature Communications</i> , 2015, 6, 6342.	12.8	761
21	Metabolic Phenotyping in Health and Disease. <i>Cell</i> , 2008, 134, 714-717.	28.9	711
22	Symbiotic Bacterial Metabolites Regulate Gastrointestinal Barrier Function via the Xenobiotic Sensor PXR and Toll-like Receptor 4. <i>Immunity</i> , 2014, 41, 296-310.	14.3	708
23	Pharmacometabonomic identification of a significant host-microbiome metabolic interaction affecting human drug metabolism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 14728-14733.	7.1	665
24	Gut microbiota modulation of chemotherapy efficacy and toxicity. <i>Nature Reviews Gastroenterology and Hepatology</i> , 2017, 14, 356-365.	17.8	643
25	Systemic gut microbial modulation of bile acid metabolism in host tissue compartments. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 4523-4530.	7.1	625
26	Preparing for Precision Medicine. <i>New England Journal of Medicine</i> , 2012, 366, 489-491.	27.0	579
27	High resolution proton magnetic resonance spectroscopy of biological fluids. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 1989, 21, 449-501.	7.5	570
28	Evaluation of the Orthogonal Projection on Latent Structure Model Limitations Caused by Chemical Shift Variability and Improved Visualization of Biomarker Changes in <sup>1</sup> H NMR Spectroscopic Metabonomic Studies. <i>Analytical Chemistry</i> , 2005, 77, 517-526.	6.5	553
29	Gut microbiome-host interactions in health and disease. <i>Genome Medicine</i> , 2011, 3, 14.	8.2	550
30	Improved WATERGATE Pulse Sequences for Solvent Suppression in NMR Spectroscopy. <i>Journal of Magnetic Resonance</i> , 1998, 132, 125-129.	2.1	518
31	Intraoperative Tissue Identification Using Rapid Evaporative Ionization Mass Spectrometry. <i>Science Translational Medicine</i> , 2013, 5, 194ra93.	12.4	488
32	Molecular phenomics and metagenomics of hepatic steatosis in non-diabetic obese women. <i>Nature Medicine</i> , 2018, 24, 1070-1080.	30.7	465
33	Integrated Metabonomic Analysis of the Multiorgan Effects of Hydrazine Toxicity in the Rat. <i>Chemical Research in Toxicology</i> , 2005, 18, 115-122.	3.3	464
34	Understanding the role of gut microbiome—host metabolic signal disruption in health and disease. <i>Trends in Microbiology</i> , 2011, 19, 349-359.	7.7	452
35	Metabolic phenotyping in clinical and surgical environments. <i>Nature</i> , 2012, 491, 384-392.	27.8	450
36	Gut microbiome interactions with drug metabolism, efficacy, and toxicity. <i>Translational Research</i> , 2017, 179, 204-222.	5.0	439

#	ARTICLE	IF	CITATIONS
37	Scaling and Normalization Effects in NMR Spectroscopic Metabonomic Data Sets. <i>Analytical Chemistry</i> , 2006, 78, 2262-2267.	6.5	438
38	Gut Microbiota Composition and Activity in Relation to Host Metabolic Phenotype and Disease Risk. <i>Cell Metabolism</i> , 2012, 16, 559-564.	16.2	438
39	UPLC/MSE; a new approach for generating molecular fragment information for biomarker structure elucidation. <i>Rapid Communications in Mass Spectrometry</i> , 2006, 20, 1989-1994.	1.5	434
40	Gut microbiota: a potential new territory for drug targeting. <i>Nature Reviews Drug Discovery</i> , 2008, 7, 123-129.	46.4	426
41	Metabonomics technologies and their applications in physiological monitoring, drug safety assessment and disease diagnosis. <i>Biomarkers</i> , 2004, 9, 1-31.	1.9	425
42	NMR-based metabonomic approaches for evaluating physiological influences on biofluid composition. <i>NMR in Biomedicine</i> , 2005, 18, 143-162.	2.8	425
43	High Resolution “Ultra Performance” Liquid Chromatography Coupled to oa-TOF Mass Spectrometry as a Tool for Differential Metabolic Pathway Profiling in Functional Genomic Studies. <i>Journal of Proteome Research</i> , 2005, 4, 591-598.	3.7	423
44	A top-down systems biology view of microbiome-mammalian metabolic interactions in a mouse model. <i>Molecular Systems Biology</i> , 2007, 3, 112.	7.2	420
45	Precision High-Throughput Proton NMR Spectroscopy of Human Urine, Serum, and Plasma for Large-Scale Metabolic Phenotyping. <i>Analytical Chemistry</i> , 2014, 86, 9887-9894.	6.5	419
46	Metabolic Profiling of Human Colorectal Cancer Using High-Resolution Magic Angle Spinning Nuclear Magnetic Resonance (HR-MAS NMR) Spectroscopy and Gas Chromatography Mass Spectrometry (GC/MS). <i>Journal of Proteome Research</i> , 2009, 8, 352-361.	3.7	414
47	Metabonomics: Metabolic processes studied by NMR spectroscopy of biofluids. <i>Concepts in Magnetic Resonance</i> , 2000, 12, 289-320.	1.3	401
48	Probiotic modulation of symbiotic gut microbial-host metabolic interactions in a humanized microbiome mouse model. <i>Molecular Systems Biology</i> , 2008, 4, 157.	7.2	392
49	Metabolic surgery profoundly influences gut microbial-host metabolic cross-talk. <i>Gut</i> , 2011, 60, 1214-1223.	12.1	391
50	Pattern recognition methods and applications in biomedical magnetic resonance. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2001, 39, 1-40.	7.5	384
51	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.	2.8	374
52	High-resolution magic-angle-spinning NMR spectroscopy for metabolic profiling of intact tissues. <i>Nature Protocols</i> , 2010, 5, 1019-1032.	12.0	355
53	The challenges of modeling mammalian biocomplexity. <i>Nature Biotechnology</i> , 2004, 22, 1268-1274.	17.5	351
54	Quantifying Diet-Induced Metabolic Changes of the Human Gut Microbiome. <i>Cell Metabolism</i> , 2015, 22, 320-331.	16.2	345

#	ARTICLE	IF	CITATIONS
55	Colonization-Induced Host-Gut Microbial Metabolic Interaction. MBio, 2011, 2, e00271-10.	4.1	342
56	Susceptibility of Human Metabolic Phenotypes to Dietary Modulation. Journal of Proteome Research, 2006, 5, 2780-2788.	3.7	337
57	Assessment of Analytical Reproducibility of <sup>1</sup> H NMR Spectroscopy Based Metabonomics for Large-Scale Epidemiological Research: the INTERMAP Study. Analytical Chemistry, 2006, 78, 2199-2208.	6.5	332
58	Statistical Heterospectroscopy, an Approach to the Integrated Analysis of NMR and UPLC-MS Data Sets: Application in Metabonomic Toxicology Studies. Analytical Chemistry, 2006, 78, 363-371.	6.5	330
59	Global systems biology, personalized medicine and molecular epidemiology. Molecular Systems Biology, 2006, 2, 52.	7.2	328
60	Microbiome-host systems interactions: protective effects of propionate upon the blood-brain barrier. Microbiome, 2018, 6, 55.	11.1	324
61	Cervical intraepithelial neoplasia disease progression is associated with increased vaginal microbiome diversity. Scientific Reports, 2015, 5, 16865.	3.3	320
62	NMR Spectroscopy of Biofluids. Annual Reports on NMR Spectroscopy, 1999, 38, 1-88.	1.5	314
63	Dietary Modulation of Gut Microbiota Contributes to Alleviation of Both Genetic and Simple Obesity in Children. EBioMedicine, 2015, 2, 968-984.	6.1	306
64	Systemic multicompartamental effects of the gut microbiome on mouse metabolic phenotypes. Molecular Systems Biology, 2008, 4, 219.	7.2	304
65	Recursive Segment-Wise Peak Alignment of Biological <sup>1</sup> H NMR Spectra for Improved Metabolic Biomarker Recovery. Analytical Chemistry, 2009, 81, 56-66.	6.5	303
66	An NMR-based metabonomic approach to investigate the biochemical consequences of genetic strain differences: application to the C57BL10J and Alpk:ApfCD mouse. FEBS Letters, 2000, 484, 169-174.	2.8	291
67	NMR-Based Metabolic Profiling and Metabonomic Approaches to Problems in Molecular Toxicology. Chemical Research in Toxicology, 2008, 21, 9-27.	3.3	289
68	Use of high-resolution proton nuclear magnetic resonance spectroscopy for rapid multi-component analysis of urine. Clinical Chemistry, 1984, 30, 426-432.	3.2	286
69	Proton-nuclear-magnetic-resonance studies of serum, plasma and urine from fasting normal and diabetic subjects. Biochemical Journal, 1984, 217, 365-375.	3.7	283
70	Chemometric Models for Toxicity Classification Based on NMR Spectra of Biofluids. Chemical Research in Toxicology, 2000, 13, 471-478.	3.3	277
71	The Consortium for Metabonomic Toxicology (COMET): aims, activities and achievements. Pharmacogenomics, 2005, 6, 691-699.	1.3	277
72	Urinary Metabolic Phenotyping Differentiates Children with Autism from Their Unaffected Siblings and Age-Matched Controls. Journal of Proteome Research, 2010, 9, 2996-3004.	3.7	277

#	ARTICLE	IF	CITATIONS
73	Nuclear Magnetic Resonance Spectroscopic and Principal Components Analysis Investigations into Biochemical Effects of Three Model Hepatotoxins. <i>Chemical Research in Toxicology</i> , 1998, 11, 260-272.	3.3	276
74	The gut microbiota influences skeletal muscle mass and function in mice. <i>Science Translational Medicine</i> , 2019, 11, .	12.4	271
75	Spectroscopic and Statistical Techniques for Information Recovery in Metabonomics and Metabolomics. <i>Annual Review of Analytical Chemistry</i> , 2008, 1, 45-69.	5.4	270
76	The Footprints of Gut Microbialâ€Mammalian Co-Metabolism. <i>Journal of Proteome Research</i> , 2011, 10, 5512-5522.	3.7	268
77	The interaction between vaginal microbiota, cervical length, and vaginal progesterone treatment for preterm birth risk. <i>Microbiome</i> , 2017, 5, 6.	11.1	266
78	Metabonomic investigations in mice infected with <i>Schistosoma mansoni</i> : An approach for biomarker identification. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004, 101, 12676-12681.	7.1	265
79	Hippurate: The Natural History of a Mammalianâ€Microbial Cometabolite. <i>Journal of Proteome Research</i> , 2013, 12, 1527-1546.	3.7	263
80	Analytical Reproducibility in <sup>1</sup> H NMR-Based Metabonomic Urinalysis. <i>Chemical Research in Toxicology</i> , 2002, 15, 1380-1386.	3.3	261
81	Summary recommendations for standardization and reporting of metabolic analyses. <i>Nature Biotechnology</i> , 2005, 23, 833-838.	17.5	261
82	Metabonomics in pharmaceutical R&D. <i>FEBS Journal</i> , 2007, 274, 1140-1151.	4.7	258
83	Metabonomics Techniques and Applications to Pharmaceutical Research & Development. <i>Pharmaceutical Research</i> , 2006, 23, 1075-1088.	3.5	256
84	An Integrated Metabonomic Investigation of Acetaminophen Toxicity in the Mouse Using NMR Spectroscopy. <i>Chemical Research in Toxicology</i> , 2003, 16, 295-303.	3.3	245
85	A Metabonomic Strategy for the Detection of the Metabolic Effects of Chamomile ( <i>Matricaria</i> ) Tj ETQq1 1 0.784314 rgBT /Overlock 1	5.25	243
86	Metabolic Profiling of CSF: Evidence That Early Intervention May Impact on Disease Progression and Outcome in Schizophrenia. <i>PLoS Medicine</i> , 2006, 3, e327.	8.4	242
87	Optimized Preprocessing of Ultra-Performance Liquid Chromatography/Mass Spectrometry Urinary Metabolic Profiles for Improved Information Recovery. <i>Analytical Chemistry</i> , 2011, 83, 5864-5872.	6.5	240
88	High resolution <sup>1</sup> H n.m.r. studies of vertebrate blood and plasma. <i>Biochemical Journal</i> , 1983, 211, 605-615.	3.7	235
89	Objective Set of Criteria for Optimization of Sample Preparation Procedures for Ultra-High Throughput Untargeted Blood Plasma Lipid Profiling by Ultra Performance Liquid Chromatographyâ€Mass Spectrometry. <i>Analytical Chemistry</i> , 2014, 86, 5766-5774.	6.5	234
90	Metabolic profiling strategy for discovery of nutritional biomarkers: proline betaine as a marker of citrus consumption. <i>American Journal of Clinical Nutrition</i> , 2010, 92, 436-443.	4.7	231

#	ARTICLE	IF	CITATIONS
91	Longitudinal analysis reveals that delayed bystander CD8+ T cell activation and early immune pathology distinguish severe COVID-19 from mild disease. <i>Immunity</i> , 2021, 54, 1257-1275.e8.	14.3	230
92	Top-Down Systems Biology Modeling of Host Metabotype~Microbiome Associations in Obese Rodents. <i>Journal of Proteome Research</i> , 2009, 8, 2361-2375.	3.7	228
93	Impact of Analytical Bias in Metabonomic Studies of Human Blood Serum and Plasma. <i>Analytical Chemistry</i> , 2006, 78, 4307-4318.	6.5	226
94	Global urinary metabolic profiling procedures using gas chromatography~mass spectrometry. <i>Nature Protocols</i> , 2011, 6, 1483-1499.	12.0	225
95	Automatic Data Reduction and Pattern Recognition Methods for Analysis of 1H Nuclear Magnetic Resonance Spectra of Human Urine from Normal and Pathological States. <i>Analytical Biochemistry</i> , 1994, 220, 284-296.	2.4	212
96	Use of relaxation-edited one-dimensional and two dimensional nuclear magnetic resonance spectroscopy to improve detection of small metabolites in blood plasma. <i>Analytical Biochemistry</i> , 2004, 325, 260-272.	2.4	212
97	NMR Spectroscopic-Based Metabonomic Studies of Urinary Metabolite Variation in Acclimatizing Germ-Free Rats. <i>Chemical Research in Toxicology</i> , 2003, 16, 1395-1404.	3.3	211
98	Therapeutic Modulation of Microbiota-Host Metabolic Interactions. <i>Science Translational Medicine</i> , 2012, 4, 137rv6.	12.4	211
99	NMR and Pattern Recognition Studies on the Time-Related Metabolic Effects of $\pm$ -Naphthylisothiocyanate on Liver, Urine, and Plasma in the Rat:~ An Integrative Metabonomic Approach. <i>Chemical Research in Toxicology</i> , 2001, 14, 1401-1412.	3.3	204
100	Metabonomic and Microbiological Analysis of the Dynamic Effect of Vancomycin-Induced Gut Microbiota Modification in the Mouse. <i>Journal of Proteome Research</i> , 2008, 7, 3718-3728.	3.7	202
101	Vaginal dysbiosis increases risk of preterm fetal membrane rupture, neonatal sepsis and is exacerbated by erythromycin. <i>BMC Medicine</i> , 2018, 16, 9.	5.5	202
102	Cryogenic Probe 13C NMR Spectroscopy of Urine for Metabonomic Studies. <i>Analytical Chemistry</i> , 2002, 74, 4588-4593.	6.5	200
103	Development of a model for classification of toxin-induced lesions using 1H NMR spectroscopy of urine combined with pattern recognition. , 1998, 11, 235-244.		198
104	Different Levels of Polybrominated Diphenyl Ethers (PBDEs) and Chlorinated Compounds in Breast Milk from Two U.K. Regions. <i>Environmental Health Perspectives</i> , 2004, 112, 1085-1091.	6.0	198
105	Application of biofluid 1H nuclear magnetic resonance-based metabonomic techniques for the analysis of the biochemical effects of dietary isoflavones on human plasma profile. <i>Analytical Biochemistry</i> , 2003, 323, 197-204.	2.4	197
106	Objective assessment of dietary patterns by use of metabolic phenotyping: a randomised, controlled, crossover trial. <i>Lancet Diabetes and Endocrinology</i> , 2017, 5, 184-195.	11.4	194
107	Peer Reviewed: So What's the Deal with Metabonomics?. <i>Analytical Chemistry</i> , 2003, 75, 384 A-391 A.	6.5	189
108	Metabonomic Characterization of Genetic Variations in Toxicological and Metabolic Responses Using Probabilistic Neural Networks. <i>Chemical Research in Toxicology</i> , 2001, 14, 182-191.	3.3	183



#	ARTICLE	IF	CITATIONS
109	Assignment of resonances for $\alpha$ -phase <sup>TM</sup> glycoproteins in high resolution proton NMR spectra of human blood plasma. FEBS Letters, 1987, 215, 311-315.	2.8	182
110	Investigations into Biochemical Changes Due to Diurnal Variation and Estrus Cycle in Female Rats Using High-Resolution <sup>1</sup> H NMR Spectroscopy of Urine and Pattern Recognition. Analytical Biochemistry, 2001, 295, 194-202.	2.4	182
111	Metabonomic Investigations into Hydrazine Toxicity in the Rat. Chemical Research in Toxicology, 2001, 14, 975-987.	3.3	179
112	Application of chemometrics to <sup>1</sup> H NMR spectroscopic data to investigate a relationship between human serum metabolic profiles and hypertension. Analyst, The, 2003, 128, 32-36.	3.5	179
113	Urinary metabolic signatures of human adiposity. Science Translational Medicine, 2015, 7, 285ra62.	12.4	178
114	Directly coupled HPLC- <sup>1</sup> H NMR and HPLC- <sup>1</sup> H NMR-MS in pharmaceutical research and development. Biomedical Applications, 2000, 748, 233-258.	1.7	177
115	High-resolution magic angle spinning <sup>1</sup> H NMR spectroscopic studies on intact rat renal cortex and medulla. Magnetic Resonance in Medicine, 1999, 41, 1108-1118.	3.0	172
116	Species Variation in the Fecal Metabolome Gives Insight into Differential Gastrointestinal Function. Journal of Proteome Research, 2008, 7, 352-360.	3.7	170
117	Combined HPLC, NMR Spectroscopy, and Ion-Trap Mass Spectrometry with Application to the Detection and Characterization of Xenobiotic and Endogenous Metabolites in Human Urine. Analytical Chemistry, 1996, 68, 4431-4435.	6.5	169
118	Physiological variation in metabolic phenotyping and functional genomic studies: use of orthogonal signal correction and PLS-DA. FEBS Letters, 2002, 530, 191-196.	2.8	169
119	Bile Acid Profiling and Quantification in Biofluids Using Ultra-Performance Liquid Chromatography Tandem Mass Spectrometry. Analytical Chemistry, 2015, 87, 9662-9670.	6.5	166
120	Quantitative Lipoprotein Subclass and Low Molecular Weight Metabolite Analysis in Human Serum and Plasma by <sup>1</sup> H NMR Spectroscopy in a Multilaboratory Trial. Analytical Chemistry, 2018, 90, 11962-11971.	6.5	165
121	High-resolution <sup>1</sup> H and <sup>1</sup> H- <sup>13</sup> C magic angle spinning NMR spectroscopy of rat liver. Magnetic Resonance in Medicine, 2000, 44, 201-207.	3.0	164
122	Improved analysis of multivariate data by variable stability scaling: application to NMR-based metabolic profiling. Analytica Chimica Acta, 2003, 490, 265-276.	5.4	164
123	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, 4407-4422.	3.7	164
124	Integrated application of transcriptomics and metabonomics yields new insight into the toxicity due to paracetamol in the mouse. Journal of Pharmaceutical and Biomedical Analysis, 2004, 35, 93-105.	2.8	163
125	Application of chemometrics to the <sup>1</sup> H NMR spectra of apple juices: discrimination between apple varieties. Food Chemistry, 1998, 61, 207-213.	8.2	162
126	Investigations into the biochemical effects of region-specific nephrotoxins. Molecular Pharmacology, 1989, 35, 242-50.	2.3	162



#	ARTICLE	IF	CITATIONS
127	Metabonomics and its role in drug development and disease diagnosis. Expert Review of Molecular Diagnostics, 2004, 4, 189-199.	3.1	161
128	Untargeted UPLC-MS Profiling Pipeline to Expand Tissue Metabolome Coverage: Application to Cardiovascular Disease. Analytical Chemistry, 2015, 87, 4184-4193.	6.5	161
129	Optimization and Evaluation of Metabolite Extraction Protocols for Untargeted Metabolic Profiling of Liver Samples by UPLC-MS. Analytical Chemistry, 2010, 82, 7779-7786.	6.5	160
130	Human metabolic profiles are stably controlled by genetic and environmental variation. Molecular Systems Biology, 2011, 7, 525.	7.2	158
131	Novel Application of Reversed-Phase UPLC-oeTOF-MS for Lipid Analysis in Complex Biological Mixtures: A New Tool for Lipidomics. Journal of Proteome Research, 2007, 6, 552-558.	3.7	156
132	Human Metabolic Phenotypes Link Directly to Specific Dietary Preferences in Healthy Individuals. Journal of Proteome Research, 2007, 6, 4469-4477.	3.7	156
133	Metabolic Phenotyping and Systems Biology Approaches to Understanding Metabolic Syndrome and Fatty Liver Disease. Gastroenterology, 2014, 146, 46-62.	1.3	153
134	750 MHz 1H NMR spectroscopy characterisation of the complex metabolic pattern of urine from patients with inborn errors of metabolism: 2-hydroxyglutaric aciduria and maple syrup urine disease. Journal of Pharmaceutical and Biomedical Analysis, 1997, 15, 1647-1659.	2.8	152
135	Panorganismal Gut Microbiome-Host Metabolic Crosstalk. Journal of Proteome Research, 2009, 8, 2090-2105.	3.7	151
136	Biofluid 1H NMR-based metabonomic techniques in nutrition research - metabolic effects of dietary isoflavones in humans. Journal of Nutritional Biochemistry, 2005, 16, 236-244.	4.2	149
137	Use of Metabonomics to Identify Impaired Fatty Acid Metabolism as the Mechanism of a Drug-Induced Toxicity. Chemical Research in Toxicology, 2004, 17, 165-173.	3.3	148
138	Statistically Integrated Metabonomic-Proteomic Studies on a Human Prostate Cancer Xenograft Model in Mice. Journal of Proteome Research, 2006, 5, 2642-2655.	3.7	146
139	High-Resolution Diffusion and Relaxation Edited One- and Two-Dimensional 1H NMR Spectroscopy of Biological Fluids. Analytical Chemistry, 1996, 68, 3370-3376.	6.5	145
140	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.	2.4	144
141	The identification of novel biomarkers of renal toxicity using automatic data reduction techniques and PCA of proton NMR spectra of urine. Chemometrics and Intelligent Laboratory Systems, 1998, 44, 245-255.	3.5	143
142	NMR and pattern recognition studies on liver extracts and intact livers from rats treated with 1±-naphthylisothiocyanate. Biochemical Pharmacology, 2002, 64, 67-77.	4.4	143
143	Geometric Trajectory Analysis of Metabolic Responses To Toxicity Can Define Treatment Specific Profiles. Chemical Research in Toxicology, 2004, 17, 579-587.	3.3	143
144	Systems Toxicology: An Integrated Genomic, Proteomic and Metabonomic Analysis of Methapyrilene Induced Hepatotoxicity in the Rat. Journal of Proteome Research, 2006, 5, 1586-1601.	3.7	143

#	ARTICLE	IF	CITATIONS
145	NMR-based metabonomic toxicity classification: hierarchical cluster analysis and k-nearest-neighbour approaches. <i>Analytica Chimica Acta</i> , 2003, 490, 3-15.	5.4	142
146	Integrative Modeling of Quantitative Plasma Lipoprotein, Metabolic, and Amino Acid Data Reveals a Multiorgan Pathological Signature of SARS-CoV-2 Infection. <i>Journal of Proteome Research</i> , 2020, 19, 4442-4454.	3.7	142
147	Metabonomic Deconvolution Of Embedded Toxicity: Application To Thioacetamide Hepato- and Nephrotoxicity. <i>Chemical Research in Toxicology</i> , 2005, 18, 639-654.	3.3	141
148	Metabonomic Investigations of Aging and Caloric Restriction in a Life-Long Dog Study. <i>Journal of Proteome Research</i> , 2007, 6, 1846-1854.	3.7	141
149	Metabonomics in Ulcerative Colitis: Diagnostics, Biomarker Identification, And Insight into the Pathophysiology. <i>Journal of Proteome Research</i> , 2010, 9, 954-962.	3.7	141
150	Metabolic Profiling of Genetic Disorders: A Multitissue <sup>1</sup> H Nuclear Magnetic Resonance Spectroscopic and Pattern Recognition Study into Dystrophic Tissue. <i>Analytical Biochemistry</i> , 2001, 293, 16-21.	2.4	140
151	The Comparison of Plasma Deproteinization Methods for the Detection of Low-Molecular-Weight Metabolites by <sup>1</sup> H Nuclear Magnetic Resonance Spectroscopy. <i>Analytical Biochemistry</i> , 2002, 304, 220-230.	2.4	140
152	Direct quantitative trait locus mapping of mammalian metabolic phenotypes in diabetic and normoglycemic rat models. <i>Nature Genetics</i> , 2007, 39, 666-672.	21.4	140
153	The evolution of partial least squares models and related chemometric approaches in metabonomics and metabolic phenotyping. <i>Journal of Chemometrics</i> , 2010, 24, 636-649.	1.3	140
154	Urinary excretion of acetaminophen and its metabolites as studied by proton NMR spectroscopy.. <i>Clinical Chemistry</i> , 1984, 30, 1631-1636.	3.2	137
155	Direct coupling of chromatographic separations to NMR spectroscopy. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 1996, 29, 1-49.	7.5	137
156	Relationship between vaginal microbial dysbiosis, inflammation, and pregnancy outcomes in cervical cerclage. <i>Science Translational Medicine</i> , 2016, 8, 350ra102.	12.4	137
157	Nuclear magnetic resonance spectroscopy and pattern recognition analysis of the biochemical processes associated with the progression of and recovery from nephrotoxic lesions in the rat induced by mercury(II) chloride and 2-bromoethanamine. <i>Molecular Pharmacology</i> , 1992, 42, 922-30.	2.3	137
158	Pharmacometabonomics as an effector for personalized medicine. <i>Pharmacogenomics</i> , 2011, 12, 103-111.	1.3	136
159	Cadmium and mercury nephrotoxicity. <i>Nature</i> , 1983, 304, 633-635.	27.8	135
160	High-performance liquid chromatography coupled to high-field proton nuclear magnetic resonance spectroscopy: application to the urinary metabolites of ibuprofen. <i>Analytical Chemistry</i> , 1993, 65, 327-330.	6.5	135
161	HILIC-UPLC-MS for Exploratory Urinary Metabolic Profiling in Toxicological Studies. <i>Analytical Chemistry</i> , 2011, 83, 382-390.	6.5	135
162	Spatially Resolved Metabolic Phenotyping of Breast Cancer by Desorption Electrospray Ionization Mass Spectrometry. <i>Cancer Research</i> , 2015, 75, 1828-1837.	0.9	134

#	ARTICLE	IF	CITATIONS
163	Optimized Sample Handling Strategy for Metabolic Profiling of Human Feces. <i>Analytical Chemistry</i> , 2016, 88, 4661-4668.	6.5	134
164	Biochemical classification of kidney carcinoma biopsy samples using magic-angle-spinning <sup>1</sup> H nuclear magnetic resonance spectroscopy. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1998, 17, 125-132.	2.8	133
165	Dietary Modulation of Gut Functional Ecology Studied by Fecal Metabonomics. <i>Journal of Proteome Research</i> , 2010, 9, 5284-5295.	3.7	133
166	A Genome-Wide Metabolic QTL Analysis in Europeans Implicates Two Loci Shaped by Recent Positive Selection. <i>PLoS Genetics</i> , 2011, 7, e1002270.	3.5	132
167	Application of pattern recognition methods to the analysis and classification of toxicological data derived from proton nuclear magnetic resonance spectroscopy of urine. <i>Molecular Pharmacology</i> , 1991, 39, 629-42.	2.3	132
168	Melamine-Induced Renal Toxicity Is Mediated by the Gut Microbiota. <i>Science Translational Medicine</i> , 2013, 5, 172ra22.	12.4	129
169	Spectral profiles of cultured neuronal and glial cells derived from HRMAS <sup>1</sup> H NMR spectroscopy. <i>NMR in Biomedicine</i> , 2002, 15, 375-384.	2.8	128
170	Environmental Metabonomics: Applying Combination Biomarker Analysis in Earthworms at a Metal Contaminated Site. <i>Ecotoxicology</i> , 2004, 13, 797-806.	2.4	128
171	Metabolic retroconversion of trimethylamine N-oxide and the gut microbiota. <i>Microbiome</i> , 2018, 6, 73.	11.1	127
172	Global metabolic responses of mice to <i>Trypanosoma brucei brucei</i> infection. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 6127-6132.	7.1	126
173	Comparative metabonomics of differential hydrazine toxicity in the rat and mouse. <i>Toxicology and Applied Pharmacology</i> , 2005, 204, 135-151.	2.8	125
174	Analytical technologies for metabonomics and metabolomics, and multi-omic information recovery. <i>TrAC - Trends in Analytical Chemistry</i> , 2008, 27, 194-204.	11.4	125
175	Opening up the "Black Box": Metabolic phenotyping and metabolome-wide association studies in epidemiology. <i>Journal of Clinical Epidemiology</i> , 2010, 63, 970-979.	5.0	125
176	Proton NMR spectra of urine as indicators of renal damage. Mercury-induced nephrotoxicity in rats. <i>Molecular Pharmacology</i> , 1985, 27, 644-51.	2.3	125
177	Metabolic Profiling and the Metabolome-Wide Association Study: Significance Level For Biomarker Identification. <i>Journal of Proteome Research</i> , 2010, 9, 4620-4627.	3.7	123
178	Robust Data Processing and Normalization Strategy for MALDI Mass Spectrometric Imaging. <i>Analytical Chemistry</i> , 2012, 84, 1310-1319.	6.5	123
179	The human gut microbiome: Implications for future health care. <i>Current Gastroenterology Reports</i> , 2008, 10, 396-403.	2.5	122
180	Neurogenesis and longevity signaling in young germ-free mice transplanted with the gut microbiota of old mice. <i>Science Translational Medicine</i> , 2019, 11, .	12.4	122

#	ARTICLE	IF	CITATIONS
181	High-Resolution Magic Angle Spinning 1H NMR Spectroscopy of Intact Liver and Kidney: Optimization of Sample Preparation Procedures and Biochemical Stability of Tissue during Spectral Acquisition. <i>Analytical Biochemistry</i> , 2000, 282, 16-23.	2.4	121
182	Chemo-informatic strategy for imaging mass spectrometry-based hyperspectral profiling of lipid signatures in colorectal cancer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 1216-1221.	7.1	120
183	Metabolomic analysis of the consequences of cadmium exposure in <i>Silene cucubalus</i> cell cultures via 1H NMR spectroscopy and chemometrics. <i>Phytochemistry</i> , 2003, 62, 851-858.	2.9	119
184	NMR spectroscopy as a novel approach to the monitoring of renal transplant function. <i>Kidney International</i> , 1993, 43, 234-245.	5.2	118
185	Toxicological applications of magnetic resonance. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2004, 45, 109-143.	7.5	118
186	Detection of Urinary Drug Metabolite (Xenometabolome) Signatures in Molecular Epidemiology Studies via Statistical Total Correlation (NMR) Spectroscopy. <i>Analytical Chemistry</i> , 2007, 79, 2629-2640.	6.5	118
187	Deep learning and 3D-DESI imaging reveal the hidden metabolic heterogeneity of cancer. <i>Chemical Science</i> , 2017, 8, 3500-3511.	7.4	117
188	Metabolome-Wide Association Study Identifies Multiple Biomarkers that Discriminate North and South Chinese Populations at Differing Risks of Cardiovascular Disease: INTERMAP Study. <i>Journal of Proteome Research</i> , 2010, 9, 6647-6654.	3.7	116
189	High resolution magic angle spinning 1H nuclear magnetic resonance analysis of intact prostatic hyperplastic and tumour tissues. <i>Analytical Communications</i> , 1998, 35, 113-115.	2.2	114
190	Extraction, interpretation and validation of information for comparing samples in metabolic LC/MS data sets. <i>Analyst</i> , 2005, 130, 701-707.	3.5	114
191	Variation in Antibiotic-Induced Microbial Recolonization Impacts on the Host Metabolic Phenotypes of Rats. <i>Journal of Proteome Research</i> , 2011, 10, 3590-3603.	3.7	114
192	High-throughput 1H NMR-based metabolic analysis of human serum and urine for large-scale epidemiological studies: validation study. <i>International Journal of Epidemiology</i> , 2008, 37, i31-i40.	1.9	113
193	Stability and Robustness of Human Metabolic Phenotypes in Response to Sequential Food Challenges. <i>Journal of Proteome Research</i> , 2012, 11, 643-655.	3.7	113
194	Development and Application of Ultra-Performance Liquid Chromatography-TOF MS for Precision Large Scale Urinary Metabolic Phenotyping. <i>Analytical Chemistry</i> , 2016, 88, 9004-9013.	6.5	113
195	Metabolomic Strategy for the Classification and Quality Control of Phytomedicine: A Case Study of Chamomile Flower ( <i>Matricaria recutita</i> L.). <i>Planta Medica</i> , 2004, 70, 250-255.	1.3	112
196	XCMS-MRM and METLIN-MRM: a cloud library and public resource for targeted analysis of small molecules. <i>Nature Methods</i> , 2018, 15, 681-684.	19.0	112
197	A Metabolite Array Technology for Precision Medicine. <i>Analytical Chemistry</i> , 2021, 93, 5709-5717.	6.5	112
198	Pattern recognition classification of the site of nephrotoxicity based on metabolic data derived from proton nuclear magnetic resonance spectra of urine. <i>Molecular Pharmacology</i> , 1994, 46, 199-211.	2.3	112

#	ARTICLE	IF	CITATIONS
199	Assignment of <sup>1</sup> H nuclear magnetic resonance visible polyunsaturated fatty acids in BT4C gliomas undergoing ganciclovir-thymidine kinase gene therapy-induced programmed cell death. <i>Cancer Research</i> , 2003, 63, 3195-201.	0.9	111
200	Metabonomic assessment of toxicity of 4- <i>fluoroaniline</i> , 3,5- <i>difluoroaniline</i> and 2- <i>fluoro</i> -4- <i>methylaniline</i> to the earthworm <i>Eisenia veneta</i> (rosa): Identification of new endogenous biomarkers. <i>Environmental Toxicology and Chemistry</i> , 2002, 21, 1966-1972.	4.3	110
201	Experimental and Analytical Variation in Human Urine in <sup>1</sup> H NMR Spectroscopy-Based Metabolic Phenotyping Studies. <i>Analytical Chemistry</i> , 2007, 79, 5204-5211.	6.5	110
202	Coordinated multitissue transcriptional and plasma metabonomic profiles following acute caloric restriction in mice. <i>Physiological Genomics</i> , 2006, 27, 187-200.	2.3	109
203	Metabonomic Studies on the Physiological Effects of Acute and Chronic Psychological Stress in Sprague-Dawley Rats. <i>Journal of Proteome Research</i> , 2007, 6, 2080-2093.	3.7	109
204	Subtle metabolic and liver gene transcriptional changes underlie diet-induced fatty liver susceptibility in insulin-resistant mice. <i>Diabetologia</i> , 2007, 50, 1867-1879.	6.3	108
205	High-resolution magic angle spinning NMR spectroscopy: Application to biomedical studies. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2009, 55, 79-100.	7.5	108
206	Serum metabolic signatures of coronary and carotid atherosclerosis and subsequent cardiovascular disease. <i>European Heart Journal</i> , 2019, 40, 2883-2896.	2.2	107
207	The Role of Gut Microbiota in Drug Response. <i>Current Pharmaceutical Design</i> , 2009, 15, 1519-1523.	1.9	105
208	Bidirectional communication between the Aryl hydrocarbon Receptor (AhR) and the microbiome tunes host metabolism. <i>Npj Biofilms and Microbiomes</i> , 2016, 2, 16014.	6.4	105
209	Directly Coupled HPLC-NMR and Its Application to Drug Metabolism. <i>Drug Metabolism Reviews</i> , 1997, 29, 705-746.	3.6	104
210	Automatic reduction of NMR spectroscopic data for statistical and pattern recognition classification of samples. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1994, 12, 1215-1225.	2.8	103
211	<sup>1</sup> H HR-MAS NMR Spectroscopy of Tumor-Induced Local Metabolic "Field-Effects" Enables Colorectal Cancer Staging and Prognostication. <i>Journal of Proteome Research</i> , 2013, 12, 959-968.	3.7	103
212	Metabolic Assessment of Human Liver Transplants from Biopsy Samples at the Donor and Recipient Stages Using High-Resolution Magic Angle Spinning <sup>1</sup> H NMR Spectroscopy. <i>Analytical Chemistry</i> , 2005, 77, 5570-5578.	6.5	102
213	Ultra high field NMR spectroscopic studies on human seminal fluid, seminal vesicle and prostatic secretions. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1994, 12, 5-19.	2.8	101
214	An integrated reverse functional genomic and metabolic approach to understanding orotic acid-induced fatty liver. <i>Physiological Genomics</i> , 2004, 17, 140-149.	2.3	101
215	A metabolic system-wide characterisation of the pig: a model for human physiology. <i>Molecular BioSystems</i> , 2011, 7, 2577.	2.9	101
216	Application of NMR-based metabolomics to the investigation of salt stress in maize ( <i>Zea mays</i> ). <i>Phytochemical Analysis</i> , 2011, 22, 214-224.	2.4	100

#	ARTICLE	IF	CITATIONS
217	Biochemical characterisation of para-aminophenol-induced nephrotoxic lesions in the F344 rat. Archives of Toxicology, 1989, 63, 97-106.	4.2	99
218	Mistargeting of Peroxisomal EHHADH and Inherited Renal Fanconi's Syndrome. New England Journal of Medicine, 2014, 370, 129-138.	27.0	99
219	An NMR-based metabonomic approach to the investigation of coelomic fluid biochemistry in earthworms under toxic stress. FEBS Letters, 2001, 500, 31-35.	2.8	98
220	High-resolution $^1\text{H}$ NMR and magic angle spinning NMR spectroscopic investigation of the biochemical effects of 2-bromoethanamine in intact renal and hepatic tissue. Magnetic Resonance in Medicine, 2001, 45, 781-790.	3.0	98
221	Integrated Metabonomic Analysis of Bromobenzene-Induced Hepatotoxicity: A Novel Induction of 5-Oxoprolinosis. Journal of Proteome Research, 2006, 5, 1448-1459.	3.7	98
222	Use of high-resolution proton nuclear magnetic resonance spectroscopy for rapid multi-component analysis of urine. Clinical Chemistry, 1984, 30, 426-32.	3.2	98
223	In Vivo Endoscopic Tissue Identification by Rapid Evaporative Ionization Mass Spectrometry (REIMS). Angewandte Chemie - International Edition, 2015, 54, 11059-11062.	13.8	97
224	Abnormal lipid profile of dystrophic cardiac tissue as demonstrated by one- and two-dimensional magic-angle spinning $^1\text{H}$ NMR spectroscopy. Magnetic Resonance in Medicine, 2001, 46, 249-255.	3.0	96
225	Evaluation of Full-Resolution $^1\text{H}$ -Resolved $^1\text{H}$ NMR Projections of Biofluids for Metabonomics Information Retrieval and Biomarker Identification. Analytical Chemistry, 2010, 82, 1811-1821.	6.5	96
226	Analysis of biological fluids using 600 MHz proton NMR spectroscopy: Application of homonuclear two-dimensional J-resolved spectroscopy to urine and blood plasma for spectral simplification and assignment. Journal of Pharmaceutical and Biomedical Analysis, 1993, 11, 21-31.	2.8	95
227	Chemical mapping of the colorectal cancer microenvironment via MALDI imaging mass spectrometry (MALDI-MSI) reveals novel cancer-associated field effects. Molecular Oncology, 2014, 8, 39-49.	4.6	95
228	Power Analysis and Sample Size Determination in Metabolic Phenotyping. Analytical Chemistry, 2016, 88, 5179-5188.	6.5	95
229	Distinction between normal and renal cell carcinoma kidney cortical biopsy samples using pattern recognition of $^1\text{H}$ magic angle spinning (MAS) NMR spectra. NMR in Biomedicine, 2000, 13, 64-71.	2.8	94
230	NMR spectroscopy based metabonomic studies on the comparative biochemistry of the kidney and urine of the bank vole ( <i>Clethrionomys glareolus</i> ), wood mouse ( <i>Apodemus sylvaticus</i> ), white toothed shrew ( <i>Crocidura suaveolens</i> ) and the laboratory rat. Comparative Biochemistry and Physiology - B Biochemistry and Molecular Biology, 2000, 127, 357-367.	1.6	94
231	A metabonomic approach to the investigation of drug-induced phospholipidosis: an NMR spectroscopy and pattern recognition study. Biomarkers, 2000, 5, 410-423.	1.9	94
232	Metabolome, transcriptome, and bioinformatic cis-element analyses point to HNF-4 as a central regulator of gene expression during enterocyte differentiation. Physiological Genomics, 2006, 27, 141-155.	2.3	94
233	Hyperspectral Visualization of Mass Spectrometry Imaging Data. Analytical Chemistry, 2013, 85, 1415-1423.	6.5	93
234	Application of orthogonal signal correction to minimise the effects of physical and biological variation in high resolution $^1\text{H}$ NMR spectra of biofluids. Analyst, The, 2002, 127, 1283-1288.	3.5	92



#	ARTICLE	IF	CITATIONS
235	A novel methodology for in vivo endoscopic phenotyping of colorectal cancer based on real-time analysis of the mucosal lipidome: a prospective observational study of the iKnife. <i>Surgical Endoscopy and Other Interventional Techniques</i> , 2017, 31, 1361-1370.	2.4	92
236	System level metabolic effects of a <i>Schistosoma japonicum</i> infection in the Syrian hamster. <i>Molecular and Biochemical Parasitology</i> , 2006, 146, 1-9.	1.1	91
237	Phylometabonomic Patterns of Adaptation to High Fat Diet Feeding in Inbred Mice. <i>PLoS ONE</i> , 2008, 3, e1668.	2.5	91
238	Pattern recognition analysis of high resolution <sup>1</sup> H NMR spectra of urine. A nonlinear mapping approach to the classification of toxicological data. <i>NMR in Biomedicine</i> , 1990, 3, 166-172.	2.8	90
239	Choline containing metabolites during cell transfection: an insight into magnetic resonance spectroscopy detectable changes. <i>FEBS Letters</i> , 2001, 509, 263-266.	2.8	90
240	An Integrated Metabonomic Approach To Describe Temporal Metabolic Disregulation Induced in the Rat by the Model Hepatotoxin Allyl Formate. <i>Journal of Proteome Research</i> , 2006, 5, 2675-2684.	3.7	90
241	Earthworm species of the genus <i>Eisenia</i> can be phenotypically differentiated by metabolic profiling. <i>FEBS Letters</i> , 2002, 521, 115-120.	2.8	89
242	Ultra Performance Liquid Chromatography-Mass Spectrometry Profiling of Bile Acid Metabolites in Biofluids: Application to Experimental Toxicology Studies. <i>Analytical Chemistry</i> , 2010, 82, 5282-5289.	6.5	89
243	Gut Microbiota Modulate the Metabolism of Brown Adipose Tissue in Mice. <i>Journal of Proteome Research</i> , 2012, 11, 620-630.	3.7	89
244	Automatic alignment of individual peaks in large high-resolution spectral data sets. <i>Journal of Magnetic Resonance</i> , 2004, 170, 329-335.	2.1	88
245	Probing Latent Biomarker Signatures and in Vivo Pathway Activity in Experimental Disease States via Statistical Total Correlation Spectroscopy (STOCSY) of Biofluids: A Application to HgCl <sub>2</sub> Toxicity. <i>Journal of Proteome Research</i> , 2006, 5, 1313-1320.	3.7	88
246	Effects of Probiotic <i>Lactobacillus Paracasei</i> Treatment on the Host Gut Tissue Metabolic Profiles Probed via Magic-Angle-Spinning NMR Spectroscopy. <i>Journal of Proteome Research</i> , 2007, 6, 1471-1481.	3.7	88
247	<sup>1</sup> H NMR Spectroscopy-Based Interventional Metabolic Phenotyping: A Cohort Study of Rheumatoid Arthritis Patients. <i>Journal of Proteome Research</i> , 2010, 9, 4545-4553.	3.7	88
248	Statistical Correlation and Projection Methods for Improved Information Recovery from Diffusion-Edited NMR Spectra of Biological Samples. <i>Analytical Chemistry</i> , 2007, 79, 5682-5689.	6.5	87
249	Directly Coupled 800 MHz HPLC- <sup>1</sup> H NMR Spectroscopy of Urine and Its Application to the Identification of the Major Phase II Metabolites of Tolfenamic Acid. <i>Analytical Chemistry</i> , 1997, 69, 607-612.	6.5	86
250	Top-down systems biology integration of conditional prebiotic modulated transgenomic interactions in a humanized microbiome mouse model. <i>Molecular Systems Biology</i> , 2008, 4, 205.	7.2	86
251	Two-dimensional proton nuclear magnetic resonance "maps" of acetaminophen metabolites in human urine.. <i>Clinical Chemistry</i> , 1985, 31, 757-762.	3.2	85
252	Incomplete Systemic Recovery and Metabolic Phenoreversion in Post-Acute-Phase Nonhospitalized COVID-19 Patients: Implications for Assessment of Post-Acute COVID-19 Syndrome. <i>Journal of Proteome Research</i> , 2021, 20, 3315-3329.	3.7	85



#	ARTICLE	IF	CITATIONS
253	Directly Coupled High-Performance Liquid Chromatography and Nuclear Magnetic Resonance Spectroscopic with Chemometric Studies on Metabolic Variation in Spragueâ€Dawley Rats. <i>Analytical Biochemistry</i> , 2001, 291, 245-252.	2.4	84
254	Kidney lesions in pelagic seabirds with high tissue levels of cadmium and mercury. <i>Journal of Zoology</i> , 1983, 200, 99-118.	1.7	84
255	Nephrocalcinosis (Enamel Renal Syndrome) Caused by Autosomal Recessive FAM20A Mutations. <i>Nephron Physiology</i> , 2013, 122, 1-6.	1.2	84
256	Batch statistical processing of <sup>1</sup> H NMR-derived urinary spectral data. <i>Journal of Chemometrics</i> , 2002, 16, 461-468.	1.3	82
257	600 MHz <sup>1</sup> H-NMR spectroscopy of human cerebrospinal fluid: Effects of sample manipulation and assignment of resonances. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1993, 11, 651-664.	2.8	81
258	Measurement of Biomolecular Diffusion Coefficients in Blood Plasma Using Two-Dimensional <sup>1</sup> Hâ€ <sup>1</sup> H Diffusion-Edited Total-Correlation NMR Spectroscopy. <i>Analytical Chemistry</i> , 1997, 69, 1504-1509.	6.5	81
259	Systemic Perturbations in Amine and Kynurenine Metabolism Associated with Acute SARS-CoV-2 Infection and Inflammatory Cytokine Responses. <i>Journal of Proteome Research</i> , 2021, 20, 2796-2811.	3.7	81
260	Virtual Chromatographic Resolution Enhancement in Cryoflow LCâ€NMR Experiments via Statistical Total Correlation Spectroscopy. <i>Analytical Chemistry</i> , 2007, 79, 3304-3311.	6.5	79
261	High-Speed Quantitative UPLC-MS Analysis of Multiple Amines in Human Plasma and Serum via Precolumn Derivatization with 6-Aminoquinolyl- <i>N</i> -hydroxysuccinimidyl Carbamate: Application to Acetaminophen-Induced Liver Failure. <i>Analytical Chemistry</i> , 2017, 89, 2478-2487.	6.5	78
262	Microbial-Host Co-metabolites Are Prodromal Markers Predicting Phenotypic Heterogeneity in Behavior, Obesity, and Impaired Glucose Tolerance. <i>Cell Reports</i> , 2017, 20, 136-148.	6.4	78
263	Comparison of in vivo <sup>1</sup> H MRS of human brain tumours with <sup>1</sup> H HR-MAS spectroscopy of intact biopsy samples in vitro. <i>Magnetic Resonance Materials in Physics, Biology, and Medicine</i> , 1999, 8, 121-128.	2.0	77
264	Statistical Spectroscopic Tools for Biomarker Discovery and Systems Medicine. <i>Analytical Chemistry</i> , 2013, 85, 5297-5303.	6.5	77
265	Multivariate metabotyping of plasma predicts survival in patients with decompensated cirrhosis. <i>Journal of Hepatology</i> , 2016, 64, 1058-1067.	3.7	77
266	Metabolic Fingerprinting Links Oncogenic PIK3CA with Enhanced Arachidonic Acid-Derived Eicosanoids. <i>Cell</i> , 2020, 181, 1596-1611.e27.	28.9	77
267	Toxicity classification from metabonomic data using a density superposition approach: â€CLOUDSâ€™. <i>Analytica Chimica Acta</i> , 2003, 490, 109-122.	5.4	76
268	Transgenomic Metabolic Interactions in a Mouse Disease Model:â€ Interactions of <i>Trichinella spiralis</i> Infection with Dietary <i>Lactobacillus paracasei</i> Supplementation. <i>Journal of Proteome Research</i> , 2006, 5, 2185-2193.	3.7	76
269	Experimental Metabonomic Model of Dietary Variation and Stress Interactions. <i>Journal of Proteome Research</i> , 2006, 5, 1535-1542.	3.7	75
270	The Metabolome-Wide Association Study: A New Look at Human Disease Risk Factors. <i>Journal of Proteome Research</i> , 2008, 7, 3637-3638.	3.7	75

#	ARTICLE	IF	CITATIONS
271	2020 visions. <i>Nature</i> , 2010, 463, 26-32.	27.8	75
272	NMR-Based Metabolic Profiling Identifies Biomarkers of Liver Regeneration Following Partial Hepatectomy in the Rat. <i>Journal of Proteome Research</i> , 2010, 9, 59-69.	3.7	75
273	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.	6.5	75
274	The emergent role of metabolic phenotyping in dynamic patient stratification. <i>Expert Opinion on Drug Metabolism and Toxicology</i> , 2014, 10, 915-919.	3.3	75
275	Tryptophan-metabolizing gut microbes regulate adult neurogenesis via the aryl hydrocarbon receptor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	75
276	Generation of Ultrahigh Peak Capacity LC Separations via Elevated Temperatures and High Linear Mobile-Phase Velocities. <i>Analytical Chemistry</i> , 2006, 78, 7278-7283.	6.5	74
277	<sup>1</sup> H NMR and UPLC-MSE Statistical Heterospectroscopy: Characterization of Drug Metabolites (Xenometabolome) in Epidemiological Studies. <i>Analytical Chemistry</i> , 2008, 80, 6835-6844.	6.5	74
278	Global Metabolic Responses of NMRI Mice to an Experimental <i>Plasmodium berghei</i> Infection. <i>Journal of Proteome Research</i> , 2008, 7, 3948-3956.	3.7	74
279	Metabolic phenotyping for monitoring surgical patients. <i>Lancet, The</i> , 2011, 377, 1817-1819.	13.7	74
280	The effects of kisspeptin on $\beta$ -cell function, serum metabolites and appetite in humans. <i>Diabetes, Obesity and Metabolism</i> , 2018, 20, 2800-2810.	4.4	74
281	Curve-Fitting Method for Direct Quantitation of Compounds in Complex Biological Mixtures Using <sup>1</sup> H NMR: A Application in Metabonomic Toxicology Studies. <i>Analytical Chemistry</i> , 2005, 77, 4556-4562.	6.5	73
282	750 MHz <sup>1</sup> H-NMR spectroscopy of human blood plasma. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1993, 11, 267-276.	2.8	72
283	The biochemical profile of rat testicular tissue as measured by magic angle spinning <sup>1</sup> H NMR spectroscopy. <i>FEBS Letters</i> , 2000, 486, 225-229.	2.8	72
284	Multi-Component Metabolic Classification of Commercial Feverfew Preparations via High-Field <sup>1</sup> H-NMR Spectroscopy and Chemometrics. <i>Planta Medica</i> , 2002, 68, 734-738.	1.3	72
285	Topographical Variation in Metabolic Signatures of Human Gastrointestinal Biopsies Revealed by High-Resolution Magic-Angle Spinning <sup>1</sup> H NMR Spectroscopy. <i>Journal of Proteome Research</i> , 2007, 6, 3944-3951.	3.7	72
286	Ultrahigh-Performance Liquid Chromatography Tandem Mass Spectrometry with Electrospray Ionization Quantification of Tryptophan Metabolites and Markers of Gut Health in Serum and Plasma—Application to Clinical and Epidemiology Cohorts. <i>Analytical Chemistry</i> , 2019, 91, 5207-5216.	6.5	72
287	Solid-phase extraction chromatography and nuclear magnetic resonance spectrometry for the identification and isolation of drug metabolites in urine. <i>Analytical Chemistry</i> , 1987, 59, 2830-2832.	6.5	71
288	Metabolic Profiling of Chronic Cadmium Exposure in the Rat. <i>Chemical Research in Toxicology</i> , 2001, 14, 1428-1434.	3.3	71

#	ARTICLE	IF	CITATIONS
289	K-OPLS package: Kernel-based orthogonal projections to latent structures for prediction and interpretation in feature space. BMC Bioinformatics, 2008, 9, 106.	2.6	71
290	Sex-dependent effects on gut microbiota regulate hepatic carcinogenic outcomes. Scientific Reports, 2017, 7, 45232.	3.3	71
291	<sup>1</sup> H NMR spectroscopic investigations of tissue metabolite biomarker response to Cu II exposure in terrestrial invertebrates: identification of free histidine as a novel biomarker of exposure to copper in earthworms. Biomarkers, 1997, 2, 295-302.	1.9	70
292	Proton MRS of human prostatic fluid: Correlations between citrate, spermine, and myo-inositol levels and changes with disease. , 1997, 30, 248-255.		70
293	Cellular environment of metabolites and a metabonomic study of tamoxifen in endometrial cells using gradient high resolution magic angle spinning <sup>1</sup> H NMR spectroscopy. Biochimica Et Biophysica Acta - General Subjects, 2003, 1619, 151-158.	2.4	70
294	Metabolic shifts due to long-term caloric restriction revealed in nonhuman primates. Experimental Gerontology, 2009, 44, 356-362.	2.8	70
295	The influence of EDTA and citrate anticoagulant addition to human plasma on information recovery from NMR-based metabolic profiling studies. Molecular BioSystems, 2010, 6, 215.	2.9	70
296	Paracetamol metabolism, hepatotoxicity, biomarkers and therapeutic interventions: a perspective. Toxicology Research, 2018, 7, 347-357.	2.1	70
297	Iron status influences non-alcoholic fatty liver disease in obesity through the gut microbiome. Microbiome, 2021, 9, 104.	11.1	70
298	Use of High-Field <sup>1</sup> H NMR Spectroscopy for the Analysis of Liquid Foods. Journal of Agricultural and Food Chemistry, 1996, 44, 1483-1487.	5.2	69
299	Ethyl glucoside in human urine following dietary exposure: detection by <sup>1</sup> H NMR spectroscopy as a result of metabonomic screening of humans. Analyst, The, 2004, 129, 259.	3.5	69
300	Identifying unknown metabolites using NMR-based metabolic profiling techniques. Nature Protocols, 2020, 15, 2538-2567.	12.0	69
301	Quantitative high resolution <sup>1</sup> H NMR urinalysis studies on the biochemical effects of cadmium in the rat. Molecular Pharmacology, 1989, 36, 398-404.	2.3	69
302	Metabolic profiling of body fluids by proton NMR: Self-poisoning episodes with paracetamol (acetaminophen). Magnetic Resonance in Medicine, 1988, 6, 300-306.	3.0	67
303	Directly coupled liquid chromatography with inductively coupled plasma mass spectrometry and orthogonal acceleration time-of-flight mass spectrometry for the identification of drug metabolites in urine: application to diclofenac using chlorine and sulfur detection. Rapid Communications in Mass Spectrometry, 2000, 14, 2377-2384.	1.5	67
304	Rapid Diagnosis and Staging of Colorectal Cancer via High-Resolution Magic Angle Spinning Nuclear Magnetic Resonance (HR-MAS NMR) Spectroscopy of Intact Tissue Biopsies. Annals of Surgery, 2014, 259, 1138-1149.	4.2	67
305	Discovery and validation of urinary metabolotypes for the diagnosis of hepatocellular carcinoma in West Africans. Hepatology, 2014, 60, 1291-1301.	7.3	67
306	Metabolite Changes in BT4C Rat Gliomas Undergoing Ganciclovir-Thymidine Kinase Gene Therapy-induced Programmed Cell Death as Studied by <sup>1</sup> H NMR Spectroscopy in Vivo, ex Vivo, and in Vitro. Journal of Biological Chemistry, 2003, 278, 45915-45923.	3.4	66

#	ARTICLE	IF	CITATIONS
307	The Mechanism of Galactosamine Toxicity Revisited; A Metabonomic Study. Journal of Proteome Research, 2007, 6, 2711-2719.	3.7	66
308	How has healthcare research performance been assessed? A systematic review. Journal of the Royal Society of Medicine, 2011, 104, 251-261.	2.0	66
309	Hepatotoxin-induced hypertaurinuria: a proton NMR study. Archives of Toxicology, 1990, 64, 407-411.	4.2	65
310	Classification of toxin-induced changes in <sup>1</sup> H NMR spectra of urine using an artificial neural network. Journal of Pharmaceutical and Biomedical Analysis, 1995, 13, 205-211.	2.8	65
311	Metabolic Phenotyping of Atherosclerotic Plaques Reveals Latent Associations between Free Cholesterol and Ceramide Metabolism in Atherogenesis. Journal of Proteome Research, 2015, 14, 1389-1399.	3.7	65
312	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.	3.5	64
313	Magic Angle Spinning Proton Nuclear Magnetic Resonance Spectroscopic Analysis of Intact Kidney Tissue Samples. Analytical Communications, 1997, 34, 107-109.	2.2	63
314	Early Metabolic Adaptation in C57BL/6 Mice Resistant to High Fat Diet Induced Weight Gain Involves an Activation of Mitochondrial Oxidative Pathways. Journal of Proteome Research, 2013, 12, 1956-1968.	3.7	63
315	Detection of in vivo biomarkers of phospholipidosis using NMR-based metabonomic approaches. Magnetic Resonance in Chemistry, 2001, 39, 559-565.	1.9	62
316	Topographical Variation in Murine Intestinal Metabolic Profiles in Relation to Microbiome Speciation and Functional Ecological Activity. Journal of Proteome Research, 2009, 8, 3464-3474.	3.7	62
317	Experimental bariatric surgery in rats generates a cytotoxic chemical environment in the gut contents. Frontiers in Microbiology, 2011, 2, 183.	3.5	62
318	MetaboNetworks, an interactive Matlab-based toolbox for creating, customizing and exploring sub-networks from KEGG. Bioinformatics, 2014, 30, 893-895.	4.1	62
319	<sup>19</sup> F-NMR and directly coupled HPLC-NMR-MS investigations into the metabolism of 2-bromo-4-trifluoromethylaniline in rat: a urinary excretion balance study without the use of radiolabelling. Xenobiotica, 1998, 28, 373-388.	1.1	61
320	NMR-Based Metabonomic Studies on the Biochemical Effects of Epicatechin in the Rat. Journal of Agricultural and Food Chemistry, 2003, 51, 4139-4145.	5.2	61
321	Biochemical Characterization of Rat Intestine Development Using High-Resolution Magic-Angle-Spinning <sup>1</sup> H NMR Spectroscopy and Multivariate Data Analysis. Journal of Proteome Research, 2005, 4, 1324-1329.	3.7	61
322	The promise of metabolic phenotyping in gastroenterology and hepatology. Nature Reviews Gastroenterology and Hepatology, 2015, 12, 458-471.	17.8	61
323	NMR Spectroscopic Windows on the Systemic Effects of SARS-CoV-2 Infection on Plasma Lipoproteins and Metabolites in Relation to Circulating Cytokines. Journal of Proteome Research, 2021, 20, 1382-1396.	3.7	61
324	Cadmium-113 NMR studies of reconstituted seven-cadmium metallothionein: evidence for structural flexibility. Biochemistry, 1985, 24, 740-747.	2.5	60

#	ARTICLE	IF	CITATIONS
325	Effects of biliary cannulation and buthionine sulfoximine pretreatment on the nephrotoxicity of para-aminophenol in the Fischer 344 rat. Archives of Toxicology, 1990, 64, 14-25.	4.2	60
326	Global Metabolic Phenotyping in an Experimental Laparotomy Model of Surgical Trauma. Journal of Proteome Research, 2011, 10, 277-287.	3.7	60
327	Analysis of polar urinary metabolites for metabolic phenotyping using supercritical fluid chromatography and mass spectrometry. Journal of Chromatography A, 2016, 1449, 141-155.	3.7	60
328	Coupling of HPLC with <sup>19</sup> F- and <sup>1</sup> H-NMR spectroscopy to investigate the human urinary excretion of flurbiprofen metabolites. Journal of Pharmaceutical and Biomedical Analysis, 1993, 11, 1009-1015.	2.8	59
329	High performance liquid chromatography coupled to nuclear magnetic resonance spectroscopy and mass spectrometry applied to plant products: Identification of ecdysteroids from <i>Silene otites</i> . Chromatographia, 1999, 49, 374-378.	1.3	59
330	Directly coupled HPLC-NMR and HPLC-MS approaches for the rapid characterisation of drug metabolites in urine: application to the human metabolism of naproxen. Journal of Pharmaceutical and Biomedical Analysis, 2001, 24, 569-579.	2.8	59
331	NMR-Based Metabonomic Studies on the Biochemical Effects of Commonly Used Drug Carrier Vehicles in the Rat. Chemical Research in Toxicology, 2002, 15, 1136-1141.	3.3	59
332	An hypothesis for a mechanism underlying hepatotoxin-induced hypercreatinuria. Archives of Toxicology, 2003, 77, 208-217.	4.2	59
333	Gut microbiome modulates the toxicity of hydrazine: a metabonomic study. Molecular BioSystems, 2009, 5, 351.	2.9	59
334	2-Furoylglycine as a Candidate Biomarker of Coffee Consumption. Journal of Agricultural and Food Chemistry, 2015, 63, 8615-8621.	5.2	59
335	Evaluation of liquid chromatography coupled with high-field <sup>1</sup> H NMR spectroscopy for drug metabolite detection and characterization: The identification of paracetamol metabolites in urine and bile. NMR in Biomedicine, 1994, 7, 295-303.	2.8	58
336	Heteronuclear <sup>1</sup> H- <sup>31</sup> P Statistical Total Correlation NMR Spectroscopy of Intact Liver for Metabolic Biomarker Assignment: Application to Galactosamine-Induced Hepatotoxicity. Analytical Chemistry, 2007, 79, 8956-8966.	6.5	58
337	Robust Algorithms for Automated Chemical Shift Calibration of 1D <sup>1</sup> H NMR Spectra of Blood Serum. Analytical Chemistry, 2008, 80, 7158-7162.	6.5	58
338	Human and preclinical studies of the host-gut microbiome co-metabolite hippurate as a marker and mediator of metabolic health. Gut, 2021, 70, 2105-2114.	12.1	58
339	Targeting the Human Genome-Microbiome Axis for Drug Discovery: Inspirations from Global Systems Biology and Traditional Chinese Medicine. Journal of Proteome Research, 2012, 11, 3509-3519.	3.7	57
340	Longitudinal pharmacometabonomics for predicting patient responses to therapy: drug metabolism, toxicity and efficacy. Expert Opinion on Drug Metabolism and Toxicology, 2012, 8, 135-139.	3.3	57
341	<sup>1</sup> H NMR studies on protein binding of histidine, tyrosine and phenylalanine in blood plasma. NMR in Biomedicine, 1989, 2, 77-82.	2.8	56
342	Flow Injection Proton Nuclear Magnetic Resonance Spectroscopy Combined With Pattern Recognition Methods: Implications for Rapid Structural Studies and High Throughput Biochemical Screening. Analytical Communications, 1997, 34, 339-341.	2.2	56

#	ARTICLE	IF	CITATIONS
343	Optimization of Human Plasma <sup>1</sup> H NMR Spectroscopic Data Processing for High-Throughput Metabolic Phenotyping Studies and Detection of Insulin Resistance Related to Type 2 Diabetes. <i>Analytical Chemistry</i> , 2008, 80, 7354-7362.	6.5	56
344	Genetic algorithms for simultaneous variable and sample selection in metabonomics. <i>Bioinformatics</i> , 2009, 25, 112-118.	4.1	56
345	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.	6.5	56
346	Metabonomics: systems biology in pharmaceutical research and development. <i>Current Opinion in Molecular Therapeutics</i> , 2004, 6, 265-72.	2.8	56
347	Induction of 5-oxoprolinuria in the rat following chronic feeding with N-acetyl 4-aminophenol (paracetamol). <i>Biochemical Pharmacology</i> , 1993, 46, 953-957.	4.4	55
348	Use of <sup>1</sup> H NMR-determined diffusion coefficients to characterize lipoprotein fractions in human blood plasma. <i>Magnetic Resonance in Chemistry</i> , 2002, 40, S83-S88.	1.9	55
349	Sexual dimorphism in urinary metabolite profiles of Han Wistar rats revealed by nuclear-magnetic-resonance-based metabonomics. <i>Analytical Biochemistry</i> , 2005, 343, 195-202.	2.4	55
350	Metabolic Phenotyping of Nude and Normal (Alpk:ApfCD, C57BL10J) Mice. <i>Journal of Proteome Research</i> , 2006, 5, 378-384.	3.7	55
351	Combined proteomic and metabonomic studies in three genetic forms of the renal Fanconi syndrome. <i>American Journal of Physiology - Renal Physiology</i> , 2007, 293, F456-F467.	2.7	55
352	Kernel-based orthogonal projections to latent structures (K&OPLS). <i>Journal of Chemometrics</i> , 2007, 21, 376-385.	1.3	55
353	Temporal Metabonomic Modeling of <sup>1</sup> H-Arginine-Induced Exocrine Pancreatitis. <i>Journal of Proteome Research</i> , 2008, 7, 4435-4445.	3.7	55
354	Uroscopy in the 21st century: high-field NMR spectroscopy. <i>Nephrology Dialysis Transplantation</i> , 1997, 12, 404-417.	0.7	54
355	HPLC/ <sup>1</sup> H NMR Spectroscopic Studies of the Reactive $\pm$ -1-O-acyl Isomer Formed during Acyl Migration of S-Naproxen $\pm$ -1-O-acyl Glucuronide. <i>Chemical Research in Toxicology</i> , 2001, 14, 1363-1370.	3.3	54
356	High resolution nuclear magnetic resonance spectroscopy of biological samples as an aid to drug development. , 1987, 31, 427-479.		54
357	Characterisation of impurities in bulk drug batches of fluticasone propionate using directly coupled HPLC-NMR spectroscopy and HPLC-MS. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1997, 16, 697-705.	2.8	53
358	Directly coupled CZE-NMR and CEC-NMR spectroscopy for metabolite analysis: paracetamol metabolites in human urine. <i>Analyst</i> , 1998, 123, 2835-2837.	3.5	53
359	High-resolution magic-angle-spinning <sup>1</sup> H NMR spectroscopy reveals different responses in choline-containing metabolites upon gene therapy-induced programmed cell death in rat brain glioma. <i>NMR in Biomedicine</i> , 2005, 18, 252-259.	2.8	53
360	Heteronuclear <sup>19</sup> F- <sup>1</sup> H Statistical Total Correlation Spectroscopy as a Tool in Drug Metabolism: Study of Flucloxacillin Biotransformation. <i>Analytical Chemistry</i> , 2008, 80, 1073-1079.	6.5	53



#	ARTICLE	IF	CITATIONS
361	Identification of metabolites in human hepatic bile using 800 MHz $^1\text{H}$ NMR spectroscopy, HPLC-NMR/MS and UPLC-MS. <i>Molecular BioSystems</i> , 2009, 5, 180-190.	2.9	53
362	Technical and Biological Variation in UPLC-MS-Based Untargeted Metabolic Profiling of Liver Extracts: Application in an Experimental Toxicity Study on Galactosamine. <i>Analytical Chemistry</i> , 2011, 83, 1116-1123.	6.5	53
363	Metabotyping of Long-Lived Mice using $^1\text{H}$ NMR Spectroscopy. <i>Journal of Proteome Research</i> , 2012, 11, 2224-2235.	3.7	53
364	The Metabolite Profiles of the Obese Population Are Gender-Dependent. <i>Journal of Proteome Research</i> , 2014, 13, 4062-4073.	3.7	53
365	Ion mobility spectrometry combined with ultra performance liquid chromatography/mass spectrometry for metabolic phenotyping of urine: Effects of column length, gradient duration and ion mobility spectrometry on metabolite detection. <i>Analytica Chimica Acta</i> , 2017, 982, 1-8.	5.4	53
366	NMR spectroscopy of human post mortem cerebrospinal fluid: Distinction of Alzheimer's disease from control using pattern recognition and statistics. <i>NMR in Biomedicine</i> , 1993, 6, 163-167.	2.8	52
367	High resolution $^1\text{H}$ NMR spectroscopic studies on dynamic biochemical processes in incubated human seminal fluid samples. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 1998, 1379, 367-380.	2.4	52
368	On-flow identification of metabolites of paracetamol from human urine using directly coupled CZE-NMR and CEC-NMR spectroscopy. <i>Analytical Communications</i> , 1998, 35, 213-215.	2.2	52
369	A metabonomic investigation of hepatotoxicity using diffusion-edited $^1\text{H}$ NMR spectroscopy of blood serum. <i>Analyst</i> , 2003, 128, 814.	3.5	52
370	Statistical Search Space Reduction and Two-Dimensional Data Display Approaches for UPLC-MS in Biomarker Discovery and Pathway Analysis. <i>Analytical Chemistry</i> , 2006, 78, 4398-4408.	6.5	52
371	Data-Driven Approach for Metabolite Relationship Recovery in Biological $^1\text{H}$ NMR Data Sets Using Iterative Statistical Total Correlation Spectroscopy. <i>Analytical Chemistry</i> , 2011, 83, 2075-2082.	6.5	52
372	A prospective cohort analysis of gut microbial co-metabolism in Alaska Native and rural African people at high and low risk of colorectal cancer. <i>American Journal of Clinical Nutrition</i> , 2020, 111, 406-419.	4.7	52
373	A comparison of quantitative NMR and radiolabelling studies of the metabolism and excretion of Statilä, (3-(4-bromo-2-fluorobenzyl)-4-oxo-3H-phthalazin-1-ylacetic acid) in the rat. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2002, 28, 31-43.	2.8	51
374	Analysis of Time-Related Metabolic Fluctuations Induced by Ethionine in the Rat. <i>Journal of Proteome Research</i> , 2007, 6, 4572-4581.	3.7	51
375	Magic Angle Spinning NMR and $^1\text{H}$ - $^{31}\text{P}$ Heteronuclear Statistical Total Correlation Spectroscopy of Intact Human Gut Biopsies. <i>Analytical Chemistry</i> , 2008, 80, 1058-1066.	6.5	51
376	Intra- and inter-omic fusion of metabolic profiling data in a systems biology framework. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2010, 104, 121-131.	3.5	51
377	High-Performance Liquid Chromatography Linked to Inductively Coupled Plasma Mass Spectrometry and Orthogonal Acceleration Time-of-Flight Mass Spectrometry for the Simultaneous Detection and Identification of Metabolites of 2-Bromo-4- trifluoromethyl-[ $^{13}\text{C}$ ]-acetanilide in Rat Urine. <i>Analytical Chemistry</i> , 2001, 73, 1491-1494.	6.5	50
378	High-resolution diffusion and relaxation-edited magic angle spinning $^1\text{H}$ NMR spectroscopy of intact liver tissue. <i>Magnetic Resonance in Medicine</i> , 2003, 50, 925-930.	3.0	50



#	ARTICLE	IF	CITATIONS
379	A study of metabolic compartmentation in the rat heart and cardiac mitochondria using high-resolution magic angle spinning <sup>1</sup> H NMR spectroscopy. FEBS Letters, 2003, 553, 73-78.	2.8	50
380	An NMR-based metabonomic investigation of the toxic effects of 3-trifluoromethyl-aniline on the earthworm <i>Eisenia veneta</i> . Biomarkers, 2000, 5, 56-72.	1.9	49
381	Studies of the biochemical toxicology of uranyl nitrate in the rat. Archives of Toxicology, 1994, 68, 43-53.	4.2	48
382	Separation and characterization of components of peptide libraries using on-flow coupled HPLC-NMR spectroscopy. Magnetic Resonance in Chemistry, 1995, 33, 857-863.	1.9	48
383	Identification of the Positional Isomers of 2-Fluorobenzoic acid 1-O-Acyl Glucuronide by Directly Coupled HPLC-NMR. Analytical Chemistry, 1995, 67, 3401-3404.	6.5	48
384	Quantitative studies on the urinary metabolic fate of 2-chloro-4-trifluoromethylaniline in the rat using <sup>19</sup> F-NMR spectroscopy and directly coupled HPLC-NMR-MS. Xenobiotica, 1999, 29, 77-91.	1.1	48
385	Metabolic Profiling of the Effects of d-Galactosamine in Liver Spheroids Using <sup>1</sup> H NMR and MAS-NMR Spectroscopy. Chemical Research in Toxicology, 2002, 15, 1351-1359.	3.3	48
386	Metabolic profiling of rodent biological fluids via <sup>1</sup> H NMR spectroscopy using a 1 mm microlitre probe. Analyst, The, 2002, 127, 582-584.	3.5	48
387	Metabolic trajectory characterisation of xenobiotic-induced hepatotoxic lesions using statistical batch processing of NMR data. Analyst, The, 2002, 127, 271-276.	3.5	48
388	Characterization of the biochemical effects of 1-nitronaphthalene in rats using global metabolic profiling by NMR spectroscopy and pattern recognition. Biomarkers, 2005, 10, 401-416.	1.9	48
389	Bariatric Surgery Modulates Circulating and Cardiac Metabolites. Journal of Proteome Research, 2014, 13, 570-580.	3.7	48
390	An Analytical Pipeline for Quantitative Characterization of Dietary Intake: Application To Assess Grape Intake. Journal of Agricultural and Food Chemistry, 2016, 64, 2423-2431.	5.2	48
391	Solid phase extraction chromatography and NMR spectroscopy (SPEC-NMR) for the rapid identification of drug metabolites in urine. Journal of Pharmaceutical and Biomedical Analysis, 1988, 6, 151-165.	2.8	47
392	The initial pathogenesis of cadmium induced renal toxicity. FEBS Letters, 2000, 478, 147-150.	2.8	47
393	Integrated Metabonomic-Proteomic Analysis of an Insect-Bacterial Symbiotic System. Journal of Proteome Research, 2010, 9, 1257-1267.	3.7	47
394	<sup>1</sup> H NMR studies of urine during fasting: Excretion of ketone bodies and acetylcarnitine. Magnetic Resonance in Medicine, 1986, 3, 849-856.	3.0	46
395	Gastro-intestinal availability of aluminium from tea. Food and Chemical Toxicology, 1993, 31, 449-454.	3.6	46
396	Analysis of Drug-Protein Binding Using Nuclear Magnetic Resonance Based Molecular Diffusion Measurements. Analytical Communications, 1997, 34, 225-228.	2.2	46

#	ARTICLE	IF	CITATIONS
397	Microbialâ€‘Mammalian Cometabolites Dominate the Age-associated Urinary Metabolic Phenotype in Taiwanese and American Populations. <i>Journal of Proteome Research</i> , 2013, 12, 3166-3180.	3.7	46
398	Integrated Analytical and Statistical Two-Dimensional Spectroscopy Strategy for Metabolite Identification: Application to Dietary Biomarkers. <i>Analytical Chemistry</i> , 2017, 89, 3300-3309.	6.5	46
399	Characterization of metabolic responses to healthy diets and association with blood pressure: application to the Optimal Macronutrient Intake Trial for Heart Health (OmniHeart), a randomized controlled study. <i>American Journal of Clinical Nutrition</i> , 2018, 107, 323-334.	4.7	46
400	750-MHz directly coupled HPLC-NMR: Application for the sequential characterization of the positional isomers and anomers of 2-, 3-, and 4-fluorobenzoic acid glucuronides in equilibrium mixtures. <i>Analytical Chemistry</i> , 1995, 67, 4441-4445.	6.5	45
401	High-resolution magic angle spinning <sup>1</sup> H-NMR spectroscopy studies on the renal biochemistry in the bank vole ( <i>Clethrionomys glareolus</i> ) and the effects of arsenic (As <sup>3+</sup> ) toxicity. <i>Xenobiotica</i> , 2001, 31, 377-385.	1.1	45
402	Qualitative high field <sup>1</sup> H-NMR spectroscopy for the characterization of endogenous metabolites in earthworms with biochemical biomarker potential. <i>Metabolomics</i> , 2005, 1, 123-136.	3.0	45
403	NMR Spectroscopic Studies on the in Vitro Acyl Glucuronide Migration Kinetics of Ibuprofen (( $\pm$ )-( <i>R,S</i> )-2-(4-Isobutylphenyl) Propanoic Acid), Its Metabolites, and Analogues. <i>Analytical Chemistry</i> , 2007, 79, 8720-8727.	6.5	45
404	Quantitative structure-metabolism relationships for substituted benzoic acids in the rat. <i>Biochemical Pharmacology</i> , 1992, 44, 1935-1946.	4.4	44
405	Proton NMR spectroscopic studies on the metabolism and biochemical effects of hydrazine in vivo. <i>Archives of Toxicology</i> , 1992, 66, 489-495.	4.2	44
406	Application of directly coupled LCâ€‘NMRâ€‘MS to the structural elucidation of metabolites of the HIV-1 reverse-transcriptase inhibitor BW935U83. <i>Biomedical Applications</i> , 2000, 748, 269-279.	1.7	44
407	Hepatotoxin-induced hypercreatinemia and hypercreatinuria: their relationship to one another, to liver damage and to weakened nutritional status. <i>Archives of Toxicology</i> , 2004, 78, 86-96.	4.2	44
408	Structural shifts of gut microbiota as surrogate endpoints for monitoring host health changes induced by carcinogen exposure. <i>FEMS Microbiology Ecology</i> , 2010, 73, no-no.	2.7	44
409	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.	6.5	44
410	Neonatal environment exerts a sustained influence on the development of the intestinal microbiota and metabolic phenotype. <i>ISME Journal</i> , 2016, 10, 145-157.	9.8	44
411	Systems parasitology: effects of <i>Fasciola hepatica</i> on the neurochemical profile in the rat brain. <i>Molecular Systems Biology</i> , 2010, 6, 396.	7.2	43
412	A metabolic phenotyping approach to understanding relationships between metabolic syndrome and breast tumour responses to chemotherapy. <i>Annals of Oncology</i> , 2012, 23, 860-866.	1.2	43
413	Diffusion and Relaxation Edited Proton NMR Spectroscopy of Plasma Reveals a High-Fidelity Supramolecular Biomarker Signature of SARS-CoV-2 Infection. <i>Analytical Chemistry</i> , 2021, 93, 3976-3986.	6.5	43
414	Urinary excretion of acetaminophen and its metabolites as studied by proton NMR spectroscopy. <i>Clinical Chemistry</i> , 1984, 30, 1631-6.	3.2	43

#	ARTICLE	IF	CITATIONS
415	Comparative studies on the nephrotoxicity of 2-bromoethanamine hydrobromide in the Fischer 344 rat and the multimammate desert mouse ( <i>Mastomys natalensis</i> ). <i>Archives of Toxicology</i> , 1995, 70, 89-95.	4.2	42
416	Analysis of fetal and neonatal urine using proton nuclear magnetic resonance spectroscopy.. <i>Archives of Disease in Childhood: Fetal and Neonatal Edition</i> , 1995, 73, F153-F157.	2.8	42
417	Dietary minerals in the gastrointestinal tract: hydroxypolymerisation of aluminium is regulated by luminal mucins. <i>Journal of Inorganic Biochemistry</i> , 1999, 75, 167-180.	3.5	42
418	High-performance liquid chromatography and inductively coupled plasma mass spectrometry (HPLC-ICP-MS) for the analysis of xenobiotic metabolites in rat urine: application to the metabolites of 4-bromoaniline. <i>Analyst, The</i> , 2000, 125, 235-236.	3.5	42
419	Vitamin E deficiency and metabolic deficits in neuronal ceroid lipofuscinosis described by bioinformatics. <i>Physiological Genomics</i> , 2002, 11, 195-203.	2.3	42
420	Variation in Gut Microbiota Strongly Influences Individual Rodent Phenotypes. <i>Toxicological Sciences</i> , 2005, 87, 1-2.	3.1	42
421	Integrated Cytokine and Metabolic Analysis of Pathological Responses to Parasite Exposure in Rodents. <i>Journal of Proteome Research</i> , 2010, 9, 2255-2264.	3.7	42
422	Development and Validation of a High-Throughput Ultrahigh-Performance Liquid Chromatography–Mass Spectrometry Approach for Screening of Oxylipins and Their Precursors. <i>Analytical Chemistry</i> , 2015, 87, 11721-11731.	6.5	42
423	Optimization and Application of Direct Infusion Nanoelectrospray HRMS Method for Large-Scale Urinary Metabolic Phenotyping in Molecular Epidemiology. <i>Journal of Proteome Research</i> , 2017, 16, 1646-1658.	3.7	42
424	Cephaloridine-induced nephrotoxicity in the Fischer 344 rat: proton NMR spectroscopic studies of urine and plasma in relation to conventional clinical chemical and histopathological assessments of nephronal damage. <i>Archives of Toxicology</i> , 1992, 66, 525-537.	4.2	41
425	Mapping the biochemical trajectory of nephrotoxicity by pattern recognition of NMR urinalysis. <i>NMR in Biomedicine</i> , 1992, 5, 368-372.	2.8	41
426	Measurement of Internal Acyl Migration Reaction Kinetics Using Directly Coupled HPLC–NMR: Application for the Positional Isomers of Synthetic (2-Fluorobenzoyl)-d-glucopyranuronic Acid. <i>Analytical Chemistry</i> , 1996, 68, 2564-2572.	6.5	41
427	Degradation of 4-Fluorobiphenyl by Mycorrhizal Fungi as Determined by <sup>19</sup> F Nuclear Magnetic Resonance Spectroscopy and <sup>14</sup> C Radiolabelling Analysis. <i>Applied and Environmental Microbiology</i> , 1999, 65, 4021-4027.	3.1	41
428	Systematic Evaluation of Extraction Methods for Multiplatform-Based Metabotyping: Application to the <i>Fasciola hepatica</i> Metabolome. <i>Analytical Chemistry</i> , 2012, 84, 6963-6972.	6.5	41
429	Nutriome–metabolome relationships provide insights into dietary intake and metabolism. <i>Nature Food</i> , 2020, 1, 426-436.	14.0	41
430	<sup>1</sup> H and <sup>2</sup> H NMR spectroscopic studies on the metabolism and biochemical effects of 2-bromoethanamine in the rat. <i>Biochemical Pharmacology</i> , 1995, 49, 1349-1359.	4.4	40
431	750 MHz HPLC–NMR Spectroscopic Studies on the Separation and Characterization of the Positional Isomers of the Glucuronides of 6,11-Dihydro-11-oxodibenz[b,e]oxepin-2-acetic Acid. <i>Analytical Chemistry</i> , 1996, 68, 106-110.	6.5	40
432	Direct observation of resolved intracellular and extracellular water signals in intact human red blood cells using <sup>1</sup> H MAS NMR spectroscopy. <i>Magnetic Resonance in Medicine</i> , 1997, 38, 334-336.	3.0	40

#	ARTICLE	IF	CITATIONS
433	Quantitative structure-metabolism relationships (QSMR) using computational chemistry: pattern recognition analysis and statistical prediction of phase II conjugation reactions of substituted benzoic acids in the rat. <i>Xenobiotica</i> , 1999, 29, 27-42.	1.1	40
434	The Influence of Pharmacogenetics on Fatty Liver Disease in the Wistar and Kyoto Rats: A Combined Transcriptomic and Metabonomic Study. <i>Journal of Proteome Research</i> , 2007, 6, 54-61.	3.7	40
435	Statistical analysis in metabolic phenotyping. <i>Nature Protocols</i> , 2021, 16, 4299-4326.	12.0	40
436	Nuclear Magnetic Resonance and High-Performance Liquid Chromatography-Nuclear Magnetic Resonance Studies on the Toxicity and Metabolism of Ifosfamide. <i>Therapeutic Drug Monitoring</i> , 1996, 18, 498-505.	2.0	40
437	Age and Microenvironment Outweigh Genetic Influence on the Zucker Rat Microbiome. <i>PLoS ONE</i> , 2014, 9, e100916.	2.5	40
438	MONITORING METABOLIC DISEASE BY PROTON NMR OF URINE. <i>Lancet, The</i> , 1984, 324, 751-752.	13.7	39
439	Acute Renal Failure Following Accidental Cutaneous Absorption of Phenol: Application of NMR Urinalysis to Monitor the Disease Process. <i>Human Toxicology</i> , 1989, 8, 491-496.	0.9	39
440	Compartmentation of metabolism probed by [2- <sup>3</sup> ]alanine: improved NMR sensitivity using a CryoProbe detects evidence of a glial metabolon. <i>Neurochemistry International</i> , 2003, 42, 93-99.	3.8	39
441	Mechanistic Aspects and Novel Biomarkers of Responder and Non-Responder Phenotypes in Galactosamine-Induced Hepatitis. <i>Journal of Proteome Research</i> , 2009, 8, 5175-5187.	3.7	39
442	Development of a Rapid Microbore Metabolic Profiling Ultrapformance Liquid Chromatography-Mass Spectrometry Approach for High-Throughput Phenotyping Studies. <i>Analytical Chemistry</i> , 2016, 88, 5742-5751.	6.5	39
443	A prospective analysis of mucosal microbiome-metabonome interactions in colorectal cancer using a combined MAS 1H NMR and metataxonomic strategy. <i>Scientific Reports</i> , 2017, 7, 8979.	3.3	39
444	Quantitative In-Vitro Diagnostic NMR Spectroscopy for Lipoprotein and Metabolite Measurements in Plasma and Serum: Recommendations for Analytical Artifact Minimization with Special Reference to COVID-19/SARS-CoV-2 Samples. <i>Journal of Proteome Research</i> , 2020, 19, 4428-4441.	3.7	39
445	19F and 1H magnetic resonance strategies for metabolic studies on fluorinated xenobiotics: Application to flurbiprofen [2-(2-fluoro-4-biphenyl)propionic acid]. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1990, 8, 401-410.	2.8	38
446	Mass spectrometrically detected directly coupled high performance liquid chromatography/nuclear magnetic resonance spectroscopy/mass spectrometry for the identification of xenobiotic metabolites in maize plants. , 2000, 14, 679-684.		38
447	Sample Classification Based on Bayesian Spectral Decomposition of Metabonomic NMR Data Sets. <i>Analytical Chemistry</i> , 2004, 76, 3666-3674.	6.5	38
448	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.	6.5	38
449	Bile UPLC-MS fingerprinting and bile acid fluxes during human liver transplantation. <i>Electrophoresis</i> , 2011, 32, 2063-2070.	2.4	38
450	Evaluation of High Resolution Magic-Angle Coil Spinning NMR Spectroscopy for Metabolic Profiling of Nanoliter Tissue Biopsies. <i>Analytical Chemistry</i> , 2012, 84, 3843-3848.	6.5	38

#	ARTICLE	IF	CITATIONS
451	Internal temperature calibration for $^1\text{H}$ NMR spectroscopy studies of blood plasma and other biofluids. <i>NMR in Biomedicine</i> , 1994, 7, 243-247.	2.8	37
452	Direct Characterization of Drug Glucuronide Isomers in Human Urine by HPLC- $^{13}\text{C}$ NMR Spectroscopy: Application to the Positional Isomers of 6,11-Dihydro-11-oxodibenz[b,e]oxepin-2-acetic Acid Glucuronide. <i>Analytical Chemistry</i> , 1996, 68, 2832-2837.	6.5	37
453	NMR Spectroscopic and Theoretical Chemistry Studies on the Internal Acyl Migration Reactions of the 1-O-Acyl- $^{12}\text{-d}_6$ -glucopyranuronate Conjugates of 2-, 3-, and 4-(Trifluoromethyl)benzoic Acids. <i>Chemical Research in Toxicology</i> , 1996, 9, 1414-1424.	3.3	37
454	Mass directed peak selection, an efficient method of drug metabolite identification using directly coupled liquid chromatography-mass spectrometry-nuclear magnetic resonance spectroscopy. <i>Biomedical Applications</i> , 2000, 748, 281-293.	1.7	37
455	Metabolism of 4-fluoroaniline and 4-fluorobiphenyl in the earthworm <i>Eisenia veneta</i> characterized by high-resolution NMR spectroscopy with directly coupled HPLC-NMR and HPLC-MS. <i>Xenobiotica</i> , 2002, 32, 479-490.	1.1	37
456	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.	6.5	37
457	Aspergillosis of the sphenoid sinus: Presentation as a pituitary mass and postoperative gallium-67 imaging. <i>World Neurosurgery</i> , 1996, 45, 354-358.	1.3	36
458	Nuclear magnetic resonance (NMR) and quantitative structure-activity relationship (QSAR) studies on the transacylation reactivity of model $^{12}\text{-O}$ -acyl glucuronides. II: QSAR modelling of the reaction using both computational and experimental NMR parameters. <i>Xenobiotica</i> , 2004, 34, 889-900.	1.1	36
459	Exploration of the direct metabolic effects of mercury II chloride on the kidney of Sprague-Dawley rats using high-resolution magic angle spinning $^1\text{H}$ NMR spectroscopy of intact tissue and pattern recognition. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2006, 40, 375-381.	2.8	36
460	The Gut Microbiota as a Target for Improved Surgical Outcome and Improved Patient Care. <i>Current Pharmaceutical Design</i> , 2009, 15, 1537-1545.	1.9	36
461	Liquid chromatography-mass spectrometry methods for urinary biomarker detection in metabonomic studies with application to nutritional studies. <i>Biomedical Chromatography</i> , 2010, 24, 737-743.	1.7	36
462	Cluster Analysis Statistical Spectroscopy Using Nuclear Magnetic Resonance Generated Metabolic Data Sets from Perturbed Biological Systems. <i>Analytical Chemistry</i> , 2009, 81, 6581-6589.	6.5	36
463	Comparative tissue distribution of mercury, cadmium and zinc in three species of pelagic seabirds. <i>Comparative Biochemistry and Physiology Part C: Comparative Pharmacology</i> , 1979, 64, 61-67.	0.2	35
464	Investigation of the human metabolism of antipyrine using coupled liquid chromatography and nuclear magnetic resonance spectroscopy of urine. <i>Biomedical Applications</i> , 1993, 617, 324-328.	1.7	35
465	Selective Inverse-Detected Long-Range Heteronuclear-Resolved NMR Spectroscopy and Its Application to the Measurement of $^3\text{JCH}$ . <i>Journal of Magnetic Resonance Series B</i> , 1995, 109, 275-283.	1.6	35
466	Chemometric analysis of biofluids following toxicant induced hepatotoxicity: A metabonomic approach to distinguish the effects of 1-naphthylisothiocyanate from its products. <i>Xenobiotica</i> , 2005, 35, 839-852.	1.1	35
467	A Two-Way Interaction between Methotrexate and the Gut Microbiota of Male Sprague-Dawley Rats. <i>Journal of Proteome Research</i> , 2020, 19, 3326-3339.	3.7	35
468	Studies on the relationship between acute testicular damage and urinary and plasma creatine concentration. <i>Archives of Toxicology</i> , 1990, 64, 443-450.	4.2	34

#	ARTICLE	IF	CITATIONS
469	Liquid chromatography coupled with high-field proton NMR for profiling human urine for endogenous compounds and drug metabolites. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1992, 10, 601-605.	2.8	34
470	Quantitative structure-metabolism relationships for substituted benzoic acids in the rabbit: prediction of urinary excretion of glycine and glucuronide conjugates. <i>Xenobiotica</i> , 1996, 26, 157-176.	1.1	34
471	Characterization of Metabolites in Intact <i>Streptomyces citricolor</i> Culture Supernatants Using High-Resolution Nuclear Magnetic Resonance and Directly Coupled High-Pressure Liquid Chromatography–Nuclear Magnetic Resonance Spectroscopy. <i>Analytical Biochemistry</i> , 1999, 270, 220-230.	2.4	34
472	Comparative biochemistry and short-term starvation effects on the earthworms <i>Eisenia veneta</i> and <i>Lumbricus terrestris</i> studied by <sup>1</sup> H NMR spectroscopy and pattern recognition. <i>Soil Biology and Biochemistry</i> , 2001, 33, 1171-1180.	8.8	34
473	Panorganismal Metabolic Response Modeling of an Experimental <i>Echinostoma caproni</i> Infection in the Mouse. <i>Journal of Proteome Research</i> , 2009, 8, 3899-3911.	3.7	34
474	Implementation of Molecular Phenotyping Approaches in the Personalized Surgical Patient Journey. <i>Annals of Surgery</i> , 2012, 255, 881-889.	4.2	34
475	Pharmacometabonomic Investigation of Dynamic Metabolic Phenotypes Associated with Variability in Response to Galactosamine Hepatotoxicity. <i>Journal of Proteome Research</i> , 2012, 11, 2427-2440.	3.7	34
476	A comparison of collision cross section values obtained via travelling wave ion mobility-mass spectrometry and ultra high performance liquid chromatography-ion mobility-mass spectrometry: Application to the characterisation of metabolites in rat urine. <i>Journal of Chromatography A</i> , 2019, 1602, 386-396.	3.7	34
477	Reduced plasma levels of small HDL particles transporting fibrinolytic proteins in pulmonary arterial hypertension. <i>Thorax</i> , 2019, 74, 380-389.	5.6	34
478	High resolution proton magnetic resonance spectroscopy of cyst fluids from patients with polycystic kidney disease. <i>Biochimica Et Biophysica Acta - Molecular Basis of Disease</i> , 1992, 1138, 305-314.	3.8	33
479	High resolution NMR spectroscopic studies on the metabolism and futile deacetylation of 4-hydroxyacetanilide (paracetamol) in the rat. <i>Biochemical Pharmacology</i> , 1995, 49, 1155-1164.	4.4	33
480	Application of Directly Coupled HPLC-NMR-MS/MS to the Identification of Metabolites of 5-Trifluoromethylpyridone (2-Hydroxy-5-trifluoromethylpyridine) in Hydroponically Grown Plants. <i>Journal of Agricultural and Food Chemistry</i> , 2000, 48, 42-46.	5.2	33
481	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.	2.8	33
482	Dietary and social modulation of gut microbiota in the elderly. <i>Nature Reviews Gastroenterology and Hepatology</i> , 2012, 9, 563-564.	17.8	33
483	Pharmacometabonomic Characterization of Xenobiotic and Endogenous Metabolic Phenotypes That Account for Inter-individual Variation in Isoniazid-Induced Toxicological Response. <i>Journal of Proteome Research</i> , 2012, 11, 4630-4642.	3.7	33
484	Chiral Metabonomics: <sup>1</sup> H NMR-Based Enantiospecific Differentiation of Metabolites in Human Urine via Direct Cosolution with $\beta$ -Cyclodextrin. <i>Analytical Chemistry</i> , 2012, 84, 2868-2874.	6.5	33
485	High-Throughput Microbore UPLC–MS Metabolic Phenotyping of Urine for Large-Scale Epidemiology Studies. <i>Journal of Proteome Research</i> , 2015, 14, 2714-2721.	3.7	33
486	Diagnostic Potential of the Plasma Lipidome in Infectious Disease: Application to Acute SARS-CoV-2 Infection. <i>Metabolites</i> , 2021, 11, 467.	2.9	33



#	ARTICLE	IF	CITATIONS
487	Studies of the biochemical toxicology of uranyl nitrate in the rat. Archives of Toxicology, 1994, 68, 43-53.	4.2	33
488	Chemical-exchange and paramagnetic T2 relaxation agents for water suppression in spin-echo proton nuclear magnetic resonance spectroscopy of biological fluids. Analytical Chemistry, 1987, 59, 2885-2891.	6.5	32
489	Patients' attitudes to xenotransplantation. Lancet, The, 1997, 349, 1031.	13.7	32
490	Impurity profiling in bulk pharmaceutical batches using <sup>19</sup> F NMR spectroscopy and distinction between monomeric and dimeric impurities by NMR-based diffusion measurements. Journal of Pharmaceutical and Biomedical Analysis, 1999, 19, 511-517.	2.8	32
491	Directly Coupled Chiral HPLC- <sup>1</sup> H NMR and HPLC- <sup>13</sup> C NMR Spectroscopy as Complementary Methods for Structural and Enantiomeric Isomer Identification: Application to Atracurium Besylate. Analytical Chemistry, 1999, 71, 2838-2843.	6.5	32
492	Kinetic and J-Resolved Statistical Total Correlation NMR Spectroscopy Approaches to Structural Information Recovery in Complex Reacting Mixtures: Application to Acyl Glucuronide Intramolecular Transacylation Reactions. Analytical Chemistry, 2008, 80, 4886-4895.	6.5	32
493	Dynamic Biochemical Information Recovery in Spontaneous Human Seminal Fluid Reactions via <sup>1</sup> H NMR Kinetic Statistical Total Correlation Spectroscopy. Analytical Chemistry, 2009, 81, 288-295.	6.5	32
494	Large-Scale Human Metabolic Phenotyping and Molecular Epidemiological Studies via <sup>1</sup> H NMR Spectroscopy of Urine: Investigation of Borate Preservation. Analytical Chemistry, 2009, 81, 4847-4856.	6.5	32
495	Metabolic Phenotypes of Carotid Atherosclerotic Plaques Relate to Stroke Risk: An Exploratory Study. European Journal of Vascular and Endovascular Surgery, 2016, 52, 5-10.	1.5	32
496	A pattern recognition approach to the comparison of PMR and clinical chemical data for classification of nephrotoxicity. Journal of Pharmaceutical and Biomedical Analysis, 1990, 8, 963-968.	2.8	31
497	Identification of novel hydrazine metabolites by <sup>15</sup> N-NMR. Biochemical Pharmacology, 1991, 41, 1319-1324.	4.4	31
498	Proton NMR Spectroscopic Studies on Tissue Extracts of Invertebrate Species with Pollution Indicator Potential. Comparative Biochemistry and Physiology - B Biochemistry and Molecular Biology, 1997, 118, 587-598.	1.6	31
499	Identification of phenacetin metabolites in human urine after administration of phenacetin-C <sup>2</sup> H <sub>3</sub> : Measurement of futile metabolic deacetylation via HPLC/MS-SPE-NMR and HPLC-ToF MS. Xenobiotica, 2006, 36, 615-629.	1.1	31
500	Integrative Modeling of Plasma Metabolic and Lipoprotein Biomarkers of SARS-CoV-2 Infection in Spanish and Australian COVID-19 Patient Cohorts. Journal of Proteome Research, 2021, 20, 4139-4152.	3.7	31
501	Metabolism of 3-chloro-4-fluoroaniline in rat using [ <sup>14</sup> C]-radiolabelling, <sup>19</sup> F-NMR spectroscopy, HPLC-MS/MS, HPLC-ICPMS and HPLC-NMR. Xenobiotica, 2006, 36, 59-77.	1.1	30
502	A Comparison of Self-Reported Analgesic Use and Detection of Urinary Ibuprofen and Acetaminophen Metabolites by Means of Metabonomics: The INTERMAP Study. American Journal of Epidemiology, 2012, 175, 348-358.	3.4	30
503	Quantitative UPLC-MS/MS analysis of the gut microbial co-metabolites phenylacetylglutamine, 4-cresyl sulphate and hippurate in human urine: INTERMAP Study. Analytical Methods, 2012, 4, 65-72.	2.7	30
504	Relation of raw and cooked vegetable consumption to blood pressure: the INTERMAP Study. Journal of Human Hypertension, 2014, 28, 353-359.	2.2	30



#	ARTICLE	IF	CITATIONS
505	mQTL.NMR: An Integrated Suite for Genetic Mapping of Quantitative Variations of <sup>1</sup> H NMR-Based Metabolic Profiles. <i>Analytical Chemistry</i> , 2015, 87, 4377-4384.	6.5	30
506	Metabolic phenotype-microRNA data fusion analysis of the systemic consequences of Roux-en-Y gastric bypass surgery. <i>International Journal of Obesity</i> , 2015, 39, 1126-1134.	3.4	30
507	BASIS: High-performance bioinformatics platform for processing of large-scale mass spectrometry imaging data in chemically augmented histology. <i>Scientific Reports</i> , 2018, 8, 4053.	3.3	30
508	The nPYc-Toolbox, a Python module for the pre-processing, quality-control and analysis of metabolic profiling datasets. <i>Bioinformatics</i> , 2019, 35, 5359-5360.	4.1	30
509	Urinary metabolic phenotyping for Alzheimer's disease. <i>Scientific Reports</i> , 2020, 10, 21745.	3.3	30
510	Studies on the comparative toxicity of S-(1,2-dichlorovinyl)-L-cysteine, S-(1,2-dichlorovinyl)-L-homocysteine and 1,1,2-trichloro-3,3,3-trifluoro-1-propene in the Fischer 344 rat. <i>Archives of Toxicology</i> , 1994, 69, 99-110.	4.2	29
511	NMR spectroscopic studies on the haemolymph of the tobacco hornworm, <i>Manduca sexta</i> : assignment of <sup>1</sup> H and <sup>13</sup> C NMR spectra. <i>Insect Biochemistry and Molecular Biology</i> , 1999, 29, 795-805.	2.7	29
512	Application of Directly Coupled HPLC NMR to Separation and Characterization of Lipoproteins from Human Serum. <i>Analytical Chemistry</i> , 2001, 73, 1084-1090.	6.5	29
513	<sup>1</sup> H NMR-based metabonomics for investigating diabetes. <i>Future Medicinal Chemistry</i> , 2009, 1, 737-747.	2.3	29
514	High Resolution <sup>1</sup> H NMR Spectroscopic Studies of the Metabolism and Excretion of Ampicillin in Rats and Amoxycillin in Rats and Man. <i>Journal of Pharmacy and Pharmacology</i> , 2011, 46, 128-134.	2.4	29
515	Genetic determinants of metabolism in health and disease: from biochemical genetics to genome-wide associations. <i>Genome Medicine</i> , 2012, 4, 30.	8.2	29
516	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.	3.7	29
517	Quantitation in gradient high performance liquid chromatography/inductively coupled mass spectrometry investigated using diclofenac and chlorpromazine. <i>Rapid Communications in Mass Spectrometry</i> , 2002, 16, 245-247.	1.5	28
518	Characterization and quantification of metabolites of racemic ketoprofen excreted in urine following oral administration to man by <sup>1</sup> H-NMR spectroscopy, directly coupled HPLC-MS and HPLC-NMR, and circular dichroism. <i>Xenobiotica</i> , 2004, 34, 1075-1089.	1.1	28
519	Integrative Top-Down System Metabolic Modeling in Experimental Disease States via Data-Driven Bayesian Methods. <i>Journal of Proteome Research</i> , 2008, 7, 497-503.	3.7	28
520	Bidirectional Correlation of NMR and Capillary Electrophoresis Fingerprints: A New Approach to Investigating <i>Schistosoma mansoni</i> Infection in a Mouse Model. <i>Analytical Chemistry</i> , 2010, 82, 203-210.	6.5	28
521	Differences in Fecal Gut Microbiota, Short-Chain Fatty Acids and Bile Acids Link Colorectal Cancer Risk to Dietary Changes Associated with Urbanization Among Zimbabweans. <i>Nutrition and Cancer</i> , 2019, 71, 1313-1324.	2.0	28
522	Two-dimensional proton nuclear magnetic resonance "maps" of acetaminophen metabolites in human urine. <i>Clinical Chemistry</i> , 1985, 31, 757-62.	3.2	28

#	ARTICLE	IF	CITATIONS
523	Integrated fecal microbiomeâ€“metabolome signatures reflect stress and serotonin metabolism in irritable bowel syndrome. <i>Gut Microbes</i> , 2022, 14, 2063016.	9.8	28
524	Spin-echo proton NMR spectroscopy of urine samples. Water suppression via a urea-DependentT2 relaxation process. <i>Magnetic Resonance in Medicine</i> , 1987, 4, 461-470.	3.0	27
525	Proton magnetic resonance spectroscopy of human urine: Excretion of 1-(3â€“carboxypropyl)-3,7-dimethylxanthine by man after dosing with oxpentifylline. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1987, 5, 157-163.	2.8	26
526	Recent advances in high-resolution NMR spectroscopic methods in bioanalytical chemistry. <i>TrAC - Trends in Analytical Chemistry</i> , 1997, 16, 190-200.	11.4	26
527	Integrated HPLC-MS and <sup>1</sup> H-NMR spectroscopic studies on acyl migration reaction kinetics of model drug ester glucuronides. <i>Xenobiotica</i> , 2010, 40, 9-23.	1.1	26
528	Use of an Atmospheric Solids Analysis Probe (ASAP) for High Throughput Screening of Biological Fluids: Preliminary Applications on Urine and Bile. <i>Journal of Proteome Research</i> , 2010, 9, 3590-3597.	3.7	26
529	Urinary Metabolic Phenotyping the slc26a6 (Chlorideâ€“Oxalate Exchanger) Null Mouse Model. <i>Journal of Proteome Research</i> , 2012, 11, 4425-4435.	3.7	26
530	Statistical Total Correlation Spectroscopy Scaling for Enhancement of Metabolic Information Recovery in Biological NMR Spectra. <i>Analytical Chemistry</i> , 2012, 84, 1083-1091.	6.5	26
531	Metabolic Phenotype Modulation by Caloric Restriction in a Lifelong Dog Study. <i>Journal of Proteome Research</i> , 2013, 12, 3117-3127.	3.7	26
532	Weaning diet induces sustained metabolic phenotype shift in the pig and influences host response to <i>Bifidobacterium lactis</i> NCC2818. <i>Gut</i> , 2013, 62, 842-851.	12.1	26
533	Roux-en-Y gastric bypass-induced bacterial perturbation contributes to altered host-bacterial co-metabolic phenotype. <i>Microbiome</i> , 2021, 9, 139.	11.1	26
534	A high resolution proton nuclear magnetic resonance approach to the study of hepatocyte and drug metabolism. Application to acetaminophen. <i>Molecular Pharmacology</i> , 1985, 27, 634-43.	2.3	26
535	Prediction of urinary sulphate and glucuronide conjugate excretion for substituted phenols in the rat using quantitative structure-metabolism relationships. <i>Xenobiotica</i> , 1995, 25, 1269-1281.	1.1	25
536	High-performance liquid chromatography directly coupled to 19F and 1H NMR for the analysis of mixtures of isomeric ester glucuronide conjugates of trifluoromethylbenzoic acids. <i>Journal of Chromatography A</i> , 1996, 728, 377-385.	3.7	25
537	NMR and HPLC-NMR spectroscopic studies of futile deacetylation in paracetamol metabolites in rat and man. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1997, 15, 901-910.	2.8	25
538	Quantitative structure-toxicity relationships for halogenated substituted-benzenes to <i>Vibrio fischeri</i> , using atom-based semi-empirical molecular-orbital descriptors. <i>Chemosphere</i> , 1999, 38, 3357-3382.	8.2	25
539	Use of directly coupled ion-exchange liquid chromatographyâ€“mass spectrometry and liquid chromatographyâ€“nuclear magnetic resonance spectroscopy as a strategy for polar metabolite identification. <i>Biomedical Applications</i> , 2000, 748, 295-309.	1.7	25
540	The potential of 19F NMR spectroscopy for rapid screening of cell cultures for models of mammalian drug metabolism. <i>Analyst</i> , The, 2001, 126, 2103-2106.	3.5	25

#	ARTICLE	IF	CITATIONS
541	LC-1H NMR used for determination of the elution order of S-naproxen glucuronide isomers in two isocratic reversed-phase LC-systems. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2001, 24, 477-485.	2.8	25
542	Synthesis, transacylation kinetics and computational chemistry of a set of arylacetic acid 1 <sup>12</sup> -O-acyl glucuronides. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 2525.	2.8	25
543	A Metabolic Entropy Approach for Measurements of Systemic Metabolic Disruptions in Patho-Physiological States. <i>Journal of Proteome Research</i> , 2010, 9, 3537-3544.	3.7	25
544	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.	3.7	25
545	Metabolic Profiling of CHO- $\alpha$ 2PP695 Cells Revealed Mitochondrial Dysfunction Prior to Amyloid- $\beta$ 2 Pathology and Potential Therapeutic Effects of Both PPAR $\beta$ 3 and PPAR $\beta$ ± Agonisms for Alzheimer's Disease. <i>Journal of Alzheimer's Disease</i> , 2015, 44, 215-231.	2.6	25
546	Proton NMR monitoring of the onset and recovery of experimental renal damage. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1990, 8, 959-962.	2.8	24
547	Application of Directly Coupled High-performance Liquid Chromatography- <sup>1</sup> H Nuclear Magnetic Resonance-Mass Spectrometry to the Detection and Characterisation of the Metabolites of 2-Bromo-4-trifluoromethylaniline in Rat Urine. <i>Analytical Communications</i> , 1997, 34, 37-39.	2.2	24
548	High-performance liquid chromatography-UV diode array, inductively coupled plasma mass spectrometry (ICMPS) and orthogonal acceleration time-of-flight mass spectrometry (oa-TOFMS) applied to the simultaneous detection and identification of metabolites of 4-bromoaniline in rat urine. <i>Chromatographia</i> , 2002, 55, S9-S13.	1.3	24
549	Self-Modeling Curve Resolution Recovery of Temporal Metabolite Signal Modulation in NMR Spectroscopic Data Sets: Application to a Life-Long Caloric Restriction Study in Dogs. <i>Analytical Chemistry</i> , 2008, 80, 4876-4885.	6.5	24
550	Piecewise multivariate modelling of sequential metabolic profiling data. <i>BMC Bioinformatics</i> , 2008, 9, 105.	2.6	24
551	A Rapid Simple Approach to Screening Pharmaceutical Products Using Ultra-Performance LC Coupled to Time-of-Flight Mass Spectrometry and Pattern Recognition. <i>Journal of Chromatographic Science</i> , 2008, 46, 193-198.	1.4	24
552	Intestinal ischemia/reperfusion injury: defining the role of the gut microbiome. <i>Biomarkers in Medicine</i> , 2009, 3, 175-192.	1.4	24
553	Dietary and Urinary Metabonomic Factors Possibly Accounting for Higher Blood Pressure of Black Compared With White Americans. <i>Hypertension</i> , 2013, 62, 1074-1080.	2.7	24
554	Application of 1 H NMR spectroscopy to the metabolic phenotyping of rodent brain extracts: A metabonomic study of gut microbial influence on host brain metabolism. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2017, 143, 141-146.	2.8	24
555	Association of Untargeted Urinary Metabolomics and Lung Cancer Risk Among Never-Smoking Women in China. <i>JAMA Network Open</i> , 2019, 2, e1911970.	5.9	24
556	Low Volume in Vitro Diagnostic Proton NMR Spectroscopy of Human Blood Plasma for Lipoprotein and Metabolite Analysis: Application to SARS-CoV-2 Biomarkers. <i>Journal of Proteome Research</i> , 2021, 20, 1415-1423.	3.7	24
557	The comparative distribution of zinc, cadmium and mercury in selected tissues of the herring gull ( <i>Larus argentatus</i> ). <i>Comparative Biochemistry and Physiology Part C: Comparative Pharmacology</i> , 1981, 68, 91-94.	0.2	23
558	Application of the one-dimensional TOCSY pulse sequence in 750 MHz 1H-NMR spectroscopy for assignment of endogenous metabolite resonances in biofluids. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1994, 12, 613-618.	2.8	23

#	ARTICLE	IF	CITATIONS
559	NMR and QSAR studies on the transacylation reactivity of model 1 <sup>2</sup> -O-acyl glucuronides. I: design, synthesis and degradation rate measurement. <i>Xenobiotica</i> , 2004, 34, 73-85.	1.1	23
560	Metabonomics in Diabetes Research. <i>Journal of Diabetes Science and Technology</i> , 2007, 1, 549-557.	2.2	23
561	Metabonomics and Metabolomics Techniques and Their Applications in Mammalian Systems. , 2007, , 1-33.		23
562	<sup>1</sup> H NMR Global Metabolic Phenotyping of Acute Pancreatitis in the Emergency Unit. <i>Journal of Proteome Research</i> , 2014, 13, 5362-5375.	3.7	23
563	Longitudinal metabolic and gut bacterial profiling of pregnant women with previous bariatric surgery. <i>Gut</i> , 2020, 69, 1452-1459.	12.1	23
564	A simultaneous exploratory and quantitative amino acid and biogenic amine metabolic profiling platform for rapid disease phenotyping via UPLC-QToF-MS. <i>Talanta</i> , 2021, 223, 121872.	5.5	23
565	Proton NMR spectroscopy of bile for monitoring the excretion of endogenous and xenobiotic metabolites: Application to para-aminophenol. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1989, 7, 699-707.	2.8	22
566	Application of Capillary Electrophoresis-Mass Spectrometry to the Analysis of Urine Samples From Animals and Man Containing Paracetamol and Phenacetin and Their Metabolites. <i>Analytical Communications</i> , 1997, 34, 41-44.	2.2	22
567	Systems biology to battle vascular disease. <i>Nephrology Dialysis Transplantation</i> , 2010, 25, 1019-1022.	0.7	22
568	<sup>1</sup> H and <sup>19</sup> F-nmr spectroscopic studies on the metabolism and urinary excretion of mono- and disubstituted phenols in the rat. <i>Xenobiotica</i> , 1996, 26, 255-273.	1.1	21
569	Studies on the metabolism of 4-fluoroaniline and 4-fluoroacetanilide in rat: formation of 4-acetamidophenol (paracetamol) and its metabolites via defluorination and N-acetylation. <i>Xenobiotica</i> , 1999, 29, 205-216.	1.1	21
570	NMR spectroscopic studies of the transacylation reactivity of ibuprofen 1 <sup>2</sup> -O-acyl glucuronide. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2006, 41, 1002-1006.	2.8	21
571	Seminal Oligouridinos: Low Uridine Secretion as a Biomarker for Infertility in Spinal Neurotrauma. <i>Clinical Chemistry</i> , 2008, 54, 2063-2066.	3.2	21
572	A Unified Conceptual Framework for Metabolic Phenotyping in Diagnosis and Prognosis. <i>Trends in Pharmacological Sciences</i> , 2019, 40, 763-773.	8.7	21
573	Untargeted Mass Spectrometry Lipidomics identifies correlation between serum sphingomyelins and plasma cholesterol. <i>Lipids in Health and Disease</i> , 2019, 18, 38.	3.0	21
574	METABONOMIC ASSESSMENT OF TOXICITY OF 4-FLUOROANILINE, 3,5-DIFLUOROANILINE AND 2-FLUORO-4-METHYLANILINE TO THE EARTHWORM EISENIA VENETA (ROSA): IDENTIFICATION OF NEW ENDOGENOUS BIOMARKERS. <i>Environmental Toxicology and Chemistry</i> , 2002, 21, 1966.	4.3	21
575	Urinary proton magnetic resonance studies of early ifosfamide-induced nephrotoxicity and encephalopathy. <i>Clinical Cancer Research</i> , 1997, 3, 1507-18.	7.0	21
576	88MHz <sup>113</sup> Cd-n.m.r. studies of native rat liver metallothioneins. <i>Biochemical Journal</i> , 1983, 211, 251-255.	3.7	20

#	ARTICLE	IF	CITATIONS
577	Quantitative structure chromatography relationships in reversed-phase high performance liquid chromatography: Prediction of retention behaviour using theoretically derived molecular properties. <i>Chromatographia</i> , 1993, 37, 241-249.	1.3	20
578	Identification of the urinary metabolites of 4-bromoaniline and 4-bromo- [carbonyl - <sup>13</sup> C]-acetanilide in rat. <i>Xenobiotica</i> , 2002, 32, 325-337.	1.1	20
579	Kinetic studies on the intramolecular acyl migration of <sup>12</sup> -1-O-acyl glucuronides: Application to the glucuronides of (R)- and (S)-ketoprofen, (R)- and (S)-hydroxy-ketoprofen metabolites, and tolmetin by 1H-NMR spectroscopy. <i>Xenobiotica</i> , 2005, 35, 715-725.	1.1	20
580	Synthesis of a series of phenylacetic acid 1- <sup>12</sup> -O-acyl glucosides and comparison of their acyl migration and hydrolysis kinetics with the corresponding acyl glucuronides. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 926-934.	2.8	20
581	MetaboSignal: a network-based approach for topological analysis of metabotype regulation <i>via</i> metabolic and signaling pathways. <i>Bioinformatics</i> , 2017, 33, 773-775.	4.1	20
582	SPUTNIK: an R package for filtering of spatially related peaks in mass spectrometry imaging data. <i>Bioinformatics</i> , 2019, 35, 178-180.	4.1	20
583	S-naproxen-beta-1-O-acyl glucuronide degradation kinetic studies by stopped-flow high-performance liquid chromatography-1H NMR and high-performance liquid chromatography-UV. <i>Drug Metabolism and Disposition</i> , 2001, 29, 375-80.	3.3	20
584	Selective Detection of 1H NMR Resonances of CH <sub>n</sub> Groups Using a Heteronuclear Maximum-Quantum Filter and Pulsed Field Gradients. <i>Journal of Magnetic Resonance Series B</i> , 1995, 106, 270-278.	1.6	19
585	Development of a simple liquid chromatographic method for the separation of mixtures of positional isomers and anomers of synthetic 2-, 3- and 4-fluorobenzoic acid glucuronides formed via acyl migration reactions. <i>Biomedical Applications</i> , 1996, 685, 113-122.	1.7	19
586	1H NMR Spectroscopic and Histopathological Studies on Propyleneimine-Induced Renal Papillary Necrosis in the Rat and the Multimammate Desert Mouse ( <i>Mastomys natalensis</i> ). <i>Comparative Biochemistry and Physiology C, Comparative Pharmacology and Toxicology</i> , 1997, 116, 125-134.	0.5	19
587	Directly-coupled HPLC-NMR spectroscopic studies of metabolism and futile deacetylation of phenacetin in the rat. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1999, 20, 865-873.	2.8	19
588	Hepatotoxin-induced hypertyrosinemia and its toxicological significance. <i>Archives of Toxicology</i> , 2007, 81, 201-210.	4.2	19
589	Broad-Ranging Natural Metabotype Variation Drives Physiological Plasticity in Healthy Control Inbred Rat Strains. <i>Journal of Proteome Research</i> , 2011, 10, 1675-1689.	3.7	19
590	Nutritional modulation of the metabonome. <i>Current Opinion in Gastroenterology</i> , 2014, 30, 196-207.	2.3	19
591	Topological analysis of metabolic networks integrating co-segregating transcriptomes and metabolomes in type 2 diabetic rat congenic series. <i>Genome Medicine</i> , 2016, 8, 101.	8.2	19
592	Ultra-Performance Liquid Chromatography-“High-Resolution Mass Spectrometry and Direct Infusion”-High-Resolution Mass Spectrometry for Combined Exploratory and Targeted Metabolic Profiling of Human Urine. <i>Journal of Proteome Research</i> , 2018, 17, 3492-3502.	3.7	19
593	Title is missing!. <i>ScienceAsia</i> , 2008, 34, 279.	0.5	19
594	Balancing the Equation: A Natural History of Trimethylamine and Trimethylamine- <i>N</i> -oxide. <i>Journal of Proteome Research</i> , 2022, 21, 560-589.	3.7	19

#	ARTICLE	IF	CITATIONS
595	Proton NMR analysis of plasma from renal failure patients: Evaluation of sample preparation and spectral-editing methods. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1990, 8, 955-958.	2.8	18
596	Recovery of Underwater Resonances by Magnetization Transferred NMR Spectroscopy (RECUR-NMR). <i>Journal of Magnetic Resonance</i> , 2001, 153, 133-137.	2.1	18
597	Bacterial adaptation to the gut environment favors successful colonization. <i>Gut Microbes</i> , 2011, 2, 307-318.	9.8	18
598	In-vitro Identification of Distinctive Metabolic Signatures of Intact Varicose Vein Tissue via Magic Angle Spinning Nuclear Magnetic Resonance Spectroscopy. <i>European Journal of Vascular and Endovascular Surgery</i> , 2012, 44, 442-450.	1.5	18
599	<i>i</i> -Resolved <sup>1</sup> H NMR 1D-Projections for Large-Scale Metabolic Phenotyping Studies: Application to Blood Plasma Analysis. <i>Analytical Chemistry</i> , 2017, 89, 11405-11412.	6.5	18
600	MWASTools: an R/bioconductor package for metabolome-wide association studies. <i>Bioinformatics</i> , 2018, 34, 890-892.	4.1	18
601	Roux-en-Y gastric bypass surgery in Zucker rats induces bacterial and systemic metabolic changes independent of caloric restriction-induced weight loss. <i>Gut Microbes</i> , 2021, 13, 1-20.	9.8	18
602	Global systems biology and personalized healthcare solutions. <i>Discovery Medicine</i> , 2006, 6, 63-70.	0.5	18
603	Selective Detection of <sup>1</sup> H NMR Resonances of <sup>13</sup> CH <sub>n</sub> Groups Using Two-Dimensional Maximum-Quantum Correlation Spectroscopy. <i>Journal of Magnetic Resonance Series A</i> , 1995, 112, 208-219.	1.6	17
604	Application of Directly Coupled High Performance Liquid Chromatography-NMR-Mass Spectrometry and <sup>1</sup> H NMR Spectroscopic Studies to the Investigation of 2,3-Benzofuran Metabolism in Sprague-Dawley Rats. <i>Drug Metabolism and Disposition</i> , 2002, 30, 1357-1363.	3.3	17
605	Reviewers peering from under a pile of "omics" data. <i>Nature</i> , 2006, 440, 992-992.	27.8	17
606	First example of hepatocyte transplantation to alleviate ornithine transcarbamylase deficiency, monitored by NMR-based metabolomics. <i>Bioanalysis</i> , 2009, 1, 1527-1535.	1.5	17
607	Metabolic Phenotype of Obesity in a Saudi Population. <i>Journal of Proteome Research</i> , 2017, 16, 635-644.	3.7	17
608	J-Edited Diffusional Proton Nuclear Magnetic Resonance Spectroscopic Measurement of Glycoprotein and Supramolecular Phospholipid Biomarkers of Inflammation in Human Serum. <i>Analytical Chemistry</i> , 2022, 94, 1333-1341.	6.5	17
609	Kidney lesions in juvenile starlings <i>Sturnus vulgaris</i> fed on a mercury-contaminated synthetic diet. <i>Environmental Pollution Series A, Ecological and Biological</i> , 1984, 33, 195-206.	0.7	16
610	Studies on the metabolism of fluorinated xenobiotics in the rat using <sup>19</sup> F-NMR and <sup>1</sup> H-NMR spectroscopy. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1990, 8, 939-944.	2.8	16
611	Proton NMR studies on the effects of uranyl nitrate on the biochemical composition of rat urine and plasma. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1990, 8, 951-954.	2.8	16
612	Chirality. <i>Analytical Proceedings</i> , 1992, 29, 225-234.	0.4	16



#	ARTICLE	IF	CITATIONS
613	Deuterium NMR spectroscopy of biofluids for the identification of drug metabolites: Application to N,N-dimethylformamide. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1993, 11, 687-692.	2.8	16
614	Determination of the relative NH proton lifetimes of the peptide analogue viomycin in aqueous solution by NMR-based diffusion measurement. <i>Journal of Biomolecular NMR</i> , 1999, 13, 25-30.	2.8	16
615	High-performance liquid chromatography/inductively coupled plasma mass spectrometry with iodine-specific detection for profiling the metabolites produced in the earthworm <i>Eisenia veneta</i> by exposure to 2-fluoro-4-iodoaniline. <i>Rapid Communications in Mass Spectrometry</i> , 2003, 17, 1855-1858.	1.5	16
616	Investigation of the metabolic fate of 2-, 3- and 4-bromobenzoic acids in bile-duct-cannulated rats by inductively coupled plasma mass spectrometry and high-performance liquid chromatography/inductively coupled plasma mass spectrometry/electrospray mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2005, 19, 519-524.	1.5	16
617	Addressing the challenge of limited sample volumes in <i>in vitro</i> studies with capillary-scale microfluidic LC-MS/MS. <i>Bioanalysis</i> , 2011, 3, 873-882.	1.5	16
618	Urinary Phenotyping Indicates Weight Loss-Independent Metabolic Effects of Roux-en-Y Gastric Bypass in Mice. <i>Journal of Proteome Research</i> , 2013, 12, 1245-1253.	3.7	16
619	Integrated Histopathological and Urinary Metabonomic Investigation of the Pathogenesis of Microcystin-LR Toxicosis. <i>Veterinary Pathology</i> , 2013, 50, 159-171.	1.7	16
620	Systemic Characterization of an Obese Phenotype in the Zucker Rat Model Defining Metabolic Axes of Energy Metabolism and Host-Microbial Interactions. <i>Journal of Proteome Research</i> , 2016, 15, 1897-1906.	3.7	16
621	A proton magnetic resonance study of the metabolism of N-methylformamide in the rat. <i>Drug Metabolism and Disposition</i> , 1986, 14, 746-9.	3.3	16
622	High-Field Deuterium Nuclear Magnetic Resonance Spectroscopic Monitoring of the Pharmacokinetics of Selectively Deuterated Benzoic Acid in Man. <i>Analytical Biochemistry</i> , 1994, 221, 297-302.	2.4	15
623	Two-dimensional $^1\text{H}$ - $^1\text{H}$ and $^{13}\text{C}$ - $^1\text{H}$ maximum-quantum correlation NMR spectroscopy with application to the assignment of the NMR spectra of the bile salt sodium taurocholate. <i>Magnetic Resonance in Chemistry</i> , 1995, 33, 212-219.	1.9	15
624	$^1\text{H}$ NMR Spectroscopic Studies on the Reactions of Haloalkylamines with Bicarbonate Ions: Formation of N-Carbamates and 2-Oxazolidones in Cell Culture Media and Blood Plasma. <i>Chemical Research in Toxicology</i> , 1995, 8, 1046-1053.	3.3	15
625	750 MHz HPLC-NMR spectroscopic identification of rat microsomal metabolites of phenoxypyridines. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1997, 16, 481-489.	2.8	15
626	Degradation of 4-fluorobiphenyl in soil investigated by $^{19}\text{F}$ NMR spectroscopy and $^{10}\text{C}$ radiolabelling analysis. <i>Chemosphere</i> , 1999, 38, 1085-1101.	8.2	15
627	$^1\text{H}$ NMR spectroscopic study of the biochemical effects of ifosfamide in the rat: evaluation of potential biomarkers. <i>Biomarkers</i> , 2000, 5, 424-435.	1.9	15
628	Investigation of the metabolism of $^{14}\text{C}/^{13}\text{C}$ -practolol in rat using directly coupled radio-HPLC-NMR-MS. <i>Xenobiotica</i> , 2000, 30, 717-729.	1.1	15
629	$^{19}\text{F}$ -NMR and directly coupled $^{19}\text{F}/^1\text{H}$ -HPLC-NMR spectroscopic investigations of the metabolism of the model ecotoxin 3-trifluoromethylaniline in the earthworm species <i>Eisenia veneta</i> . <i>Xenobiotica</i> , 2002, 32, 535-546.	1.1	15
630	An integrated ceramic, micro-fluidic device for the LC/MS/MS analysis of pharmaceuticals in plasma. <i>Analyst</i> , 2015, 140, 5546-5556.	3.5	15



#	ARTICLE	IF	CITATIONS
631	Molecular Phenomic Approaches to Deconvolving the Systemic Effects of SARS-CoV-2 Infection and Post-acute COVID-19 Syndrome. <i>Phenomics</i> , 2021, 1, 143-150.	2.9	15
632	Enhanced effect of magnetic field gradients using multiple quantum NMR spectroscopy applied to self-diffusion coefficient measurement. <i>Molecular Physics</i> , 1998, 93, 913-920.	1.7	15
633	Analysis of biological fluids by high-field nuclear magnetic resonance spectroscopy. <i>TrAC - Trends in Analytical Chemistry</i> , 1989, 8, 368-374.	11.4	14
634	<sup>1</sup> H-NMR spectroscopy of biofluids and the investigation of xenobiotic-induced changes in liver biochemistry. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1990, 8, 945-949.	2.8	14
635	NMR-monitored solid-phase extraction of phenolphthalein glucuronide on phenylboronic acid and C18 bonded phases. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1991, 9, 895-899.	2.8	14
636	Hyphenated methods. <i>Analytical Proceedings</i> , 1993, 30, 390.	0.4	14
637	Improvement in the characterization of minor drug metabolites from HPLC-NMR studies through the use of quantified maximum entropy processing of NMR spectra. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1994, 12, 419-424.	2.8	14
638	NMR spectroscopic studies on the metabolism and futile deacetylation of phenacetin in the rat. <i>Xenobiotica</i> , 1997, 27, 1175-1186.	1.1	14
639	Metabonomic investigations into the global biochemical sequelae of exposure to the pancreatic toxin 1- $\alpha$ -cyano-2-hydroxy-3-butene in the rat. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, S26-35.	1.9	14
640	Statistical HOMogeneous Cluster SpectroscopyY (SHOCSY): An Optimized Statistical Approach for Clustering of <sup>1</sup> H NMR Spectral Data to Reduce Interference and Enhance Robust Biomarkers Selection. <i>Analytical Chemistry</i> , 2014, 86, 5308-5315.	6.5	14
641	A multiplexed targeted assay for high-throughput quantitative analysis of serum methylamines by ultra performance liquid chromatography coupled to high resolution mass spectrometry. <i>Archives of Biochemistry and Biophysics</i> , 2016, 597, 12-20.	3.0	14
642	Longitudinal analysis of serum oxylipin profile as a novel descriptor of the inflammatory response to surgery. <i>Journal of Translational Medicine</i> , 2017, 15, 83.	4.4	14
643	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.	2.7	14
644	NMR studies of crab and plaice metallothioneins.. <i>Environmental Health Perspectives</i> , 1986, 65, 157-165.	6.0	13
645	Asymptomatic 5-oxoprolinuria detected by proton magnetic resonance spectroscopy. <i>Clinical Chemistry</i> , 1993, 39, 1341-1341.	3.2	13
646	Assignment of the 750 MHz <sup>1</sup> H NMR resonances from a mixture of transacylated ester glucuronic acid conjugates with the aid of oversampling and digital filtering during acquisition. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1995, 13, 971-977.	2.8	13
647	Structure-metabolism relationships of substituted anilines: prediction of N-acetylation and N-oxanilic acid formation using computational chemistry. <i>Xenobiotica</i> , 2002, 32, 267-277.	1.1	13
648	The metabolism of 4-trifluoromethoxyaniline and [13C]-4-trifluoromethoxyacetanilide in the rat: detection and identification of metabolites excreted in the urine by NMR and HPLC-NMR. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2002, 28, 875-885.	2.8	13

#	ARTICLE	IF	CITATIONS
649	Probing Molecular Dynamics in Chromatographic Systems Using High-Resolution $^1\text{H}$ Magic-Angle-Spinning NMR Spectroscopy: A Interaction between <i>p</i> -Xylene and C18-Bonded Silica. <i>Analytical Chemistry</i> , 2004, 76, 3023-3028.	6.5	13
650	UPLC/MSE; a new approach for generating molecular fragment information for biomarker structure elucidation. <i>Rapid Communications in Mass Spectrometry</i> , 2006, 20, 2234-2234.	1.5	13
651	Metabolism of 2-fluoro-4-iodoaniline in earthworm <i>Eisenia veneta</i> using $^{19}\text{F}$ -NMR spectroscopy, HPLC-MS, and HPLC-ICPMS (127I). <i>Xenobiotica</i> , 2007, 37, 1378-1393.	1.1	13
652	COMET and the Challenge of Drug Safety Screening. <i>Journal of Proteome Research</i> , 2007, 6, 4098-4099.	3.7	13
653	Application of the FLIPSY Pulse Sequence for Increased Sensitivity in $^1\text{H}$ NMR-Based Metabolic Profiling Studies. <i>Analytical Chemistry</i> , 2008, 80, 3365-3371.	6.5	13
654	Chemical shift calibration of $^1\text{H}$ MAS NMR liver tissue spectra exemplified using a study of glycine protection of galactosamine toxicity. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, S47-53.	1.9	13
655	High-performance liquid chromatography/mass spectrometric and proton nuclear magnetic resonance spectroscopic studies of the transacylation and hydrolysis of the acyl glucuronides of a series of phenylacetic acids in buffer and human plasma. <i>Rapid Communications in Mass Spectrometry</i> , 2010, 24, 3043-3051.	1.5	13
656	A novel LC-MS approach for the detection of metabolites in DMPK studies. <i>Bioanalysis</i> , 2010, 2, 1767-1778.	1.5	13
657	Non-linear modeling of $^1\text{H}$ NMR metabonomic data using kernel-based orthogonal projections to latent structures optimized by simulated annealing. <i>Analytica Chimica Acta</i> , 2011, 705, 72-80.	5.4	13
658	Urinary Metabolic Phenotyping of Women with Lower Urinary Tract Symptoms. <i>Journal of Proteome Research</i> , 2017, 16, 4208-4216.	3.7	13
659	Exploration of Human Serum Lipoprotein Supramolecular Phospholipids Using Statistical Heterospectroscopy in $n$ -Dimensions (SHY- $n$ ): Identification of Potential Cardiovascular Risk Biomarkers Related to SARS-CoV-2 Infection. <i>Analytical Chemistry</i> , 2022, 94, 4426-4436.	6.5	13
660	PROTON SPECTROSCOPY OF PLASMA AND TESTING FOR MALIGNANCY. <i>Lancet, The</i> , 1987, 330, 280-281.	13.7	12
661	Studies on the effects of $(\pm S, 5S)$ - $\beta$ -amino-3-chloro-4,5-dihydro-5-isoxazoleacetic acid (AT-125) on 4-aminophenol-induced nephrotoxicity in the Fischer 344 rat. <i>Archives of Toxicology</i> , 1993, 67, 696-705.	4.2	12
662	Comparative biochemical effects of low doses of mercury II chloride in the F344 rat and the multimammate mouse ( <i>Mastomys natalensis</i> ). <i>Comparative Biochemistry and Physiology C, Comparative Pharmacology and Toxicology</i> , 1996, 114, 7-15.	0.5	12
663	NMR spectroscopic diffusion, chemical shift and linewidth measurements of low-affinity binding of ibuprofen enantiomers to human serum albumin. <i>Magnetic Resonance in Chemistry</i> , 1999, 37, 269-273.	1.9	12
664	Identification and quantification of metabolites of 2,3,5,6-tetrafluoro-4-trifluoromethylaniline in rat urine using $^{19}\text{F}$ nuclear magnetic resonance spectroscopy, high-performance liquid chromatography- $^{19}\text{F}$ nuclear magnetic resonance spectroscopy and high-performance liquid chromatography-mass spectrometry. <i>Biomedical Applications</i> , 2000, 748, 311-319.	1.7	12
665	The metabolism of 2-trifluoromethylaniline and its acetanilide in the rat by $^{19}\text{F}$ NMR monitored enzyme hydrolysis and $^1\text{H}/^{19}\text{F}$ HPLC-NMR spectroscopy. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2003, 30, 1561-1574.	2.8	12
666	Effect of the Histone Deacetylase Inhibitor Trichostatin A on the Metabolome of Cultured Primary Hepatocytes. <i>Journal of Proteome Research</i> , 2010, 9, 413-419.	3.7	12

#	ARTICLE	IF	CITATIONS
667	pJRES Binning Algorithm (JBA): a new method to facilitate the recovery of metabolic information from pJRES 1H NMR spectra. <i>Bioinformatics</i> , 2019, 35, 1916-1922.	4.1	12
668	X-ray microanalysis of proximal and distal tubule cells in the mouse kidney, and the influence of cadmium on the concentration of natural intracellular elements. <i>Journal of Cell Science</i> , 1983, 62, 319-38.	2.0	12
669	Investigation of the quantitative metabolic fate and urinary excretion of 3-methyl-4-trifluoromethylaniline and 3-methyl-4-trifluoromethylacetanilide in the rat. <i>Drug Metabolism and Disposition</i> , 1999, 27, 1171-8.	3.3	12
670	Investigation of the feasibility of directly-coupled HPLC-NMR with 2H detection with application to the metabolism of N-dimethylformamide-d7. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1997, 16, 1-5.	2.8	11
671	Diffusion Coefficient Measurement by High Resolution NMR Spectroscopy: Biochemical and Pharmaceutical Applications. <i>Reviews in Analytical Chemistry</i> , 1999, 18, .	3.2	11
672	Peer Reviewed: Advancing Hyphenated Chromatographic Systems.. <i>Analytical Chemistry</i> , 2000, 72, 534 A-542 A.	6.5	11
673	Characterisation of putative pentose-containing conjugates as minor metabolites of 4-bromoaniline present in the urine of rats following intraperitoneal administration. <i>Rapid Communications in Mass Spectrometry</i> , 2003, 17, 76-80.	1.5	11
674	An NMR-based metabolomic approach to the analysis of the effects of xenobiotics on endogenous metabolite levels in plants. <i>Spectroscopy</i> , 2004, 18, 279-287.	0.8	11
675	Modeling Longitudinal Metabonomics and Microbiota Interactions in C57BL/6 Mice Fed a High Fat Diet. <i>Analytical Chemistry</i> , 2016, 88, 7617-7626.	6.5	11
676	The pathophysiology of human obstructive cholestasis is mimicked in cholestatic Gold Syrian hamsters. <i>Biochimica Et Biophysica Acta - Molecular Basis of Disease</i> , 2018, 1864, 942-951.	3.8	11
677	Systematic Isolation and Structure Elucidation of Urinary Metabolites Optimized for the Analytical-Scale Molecular Profiling Laboratory. <i>Analytical Chemistry</i> , 2019, 91, 8873-8882.	6.5	11
678	Systems Genetics of Hepatic Metabolome Reveals Octopamine as a Target for Non-Alcoholic Fatty Liver Disease Treatment. <i>Scientific Reports</i> , 2019, 9, 3656.	3.3	11
679	Cadmium complexes of dicysteinoethylenediaminetetraacetic acid exhibit cadmium-113 NMR shifts and cadmium-113-cadmium-113 couplings similar to those of metallothionein. <i>Journal of the American Chemical Society</i> , 1984, 106, 1118-1119.	13.7	10
680	Proton nuclear magnetic resonance of urine and bile from paracetamol dosed rats. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1990, 8, 969-973.	2.8	10
681	Raised transaminase activity of blood plasma from rats with experimentally-induced kidney damage detected by spin-echo 1H-NMR spectroscopy. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1993, 11, 897-902.	2.8	10
682	Observation of Separate J-Resolved 1H-NMR Spectra from CH, CH2, and CH3 Groups Using a Maximum-Quantum Filter. <i>Journal of Magnetic Resonance Series A</i> , 1995, 113, 251-256.	1.6	10
683	Nuclear Magnetic Resonance Spectroscopy: A Non-Invasive Probe of Kidney Metabolism and Function. <i>Nephron Experimental Nephrology</i> , 1998, 6, 409-414.	2.2	10
684	Topics in Xenobiochemistry: Do metabolic pathways exist for xenobiotics? The micro-metabolism hypothesis. <i>Xenobiotica</i> , 2003, 33, 887-901.	1.1	10

#	ARTICLE	IF	CITATIONS
685	“Omics Dreams of Personalized Healthcare. Journal of Proteome Research, 2006, 5, 2067-2069.	3.7	10
686	Modeling the effects of toxins in metabolic networks. IEEE Engineering in Medicine and Biology Magazine, 2007, 26, 37-46.	0.8	10
687	Human Metabolic Phenotyping and Metabolome Wide Association Studies. Ernst Schering Research Foundation Workshop, 2008, , 227-249.	0.7	10
688	Early intervention with Bifidobacterium lactis NCC2818 modulates the host-microbe interface independent of the sustained changes induced by the neonatal environment. Scientific Reports, 2017, 7, 5310.	3.3	10
689	Three-Dimensional Maximum-Quantum Correlation HMQC NMR Spectroscopy (3D MAXY-HMQC). Journal of Magnetic Resonance, 1997, 129, 67-73.	2.1	9
690	Quantitative urinalysis of the mercapturic acid conjugates of allyl formate using high-resolution NMR spectroscopy. Journal of Pharmaceutical and Biomedical Analysis, 2006, 40, 410-416.	2.8	9
691	Isotopic enrichment enhancement in metabonomic analysis of UPLC-MS data sets. Journal of Labelled Compounds and Radiopharmaceuticals, 2007, 50, 303-307.	1.0	9
692	A QSAR investigation of dermal and respiratory chemical sensitizers based on computational chemistry properties. SAR and QSAR in Environmental Research, 2009, 20, 429-451.	2.2	9
693	Urinary metabolites of 2-bromoethanamine identified by stable isotope labelling: evidence for carbamoylation and glutathione conjugation. Xenobiotica, 2011, 41, 144-154.	1.1	9
694	Development of a Pipeline for Exploratory Metabolic Profiling of Infant Urine. Journal of Proteome Research, 2016, 15, 3432-3440.	3.7	9
695	Improved Spatial Resolution of Metabolites in Tissue Biopsies Using High-Resolution Magic-Angle-Spinning Slice Localization NMR Spectroscopy. Analytical Chemistry, 2020, 92, 11516-11519.	6.5	9
696	Use of high-field nuclear magnetic resonance spectroscopy for the analysis of biological fluids. Analytical Proceedings, 1991, 28, 217.	0.4	8
697	Studies on the biochemical effects of the aldose reductase inhibitor 2,7-difluorospirofluorene-9,5- $\epsilon^2$ -imidazolidine-2- $\epsilon^2$ ,4- $\epsilon^2$ -dione (AI 1576, HOE 843). Biochemical Pharmacology, 1992, 44, 231-241.	4.4	8
698	Quantitative Structure-Toxicity Relationships for Halobenzenes in Two Species of Bioluminescent Bacteria, <i>Pseudomonas fluorescens</i> and <i>Vibrio fischeri</i> , Using an Atom-Centered Semi-Empirical Molecular-Orbital Based Model. SAR and QSAR in Environmental Research, 1999, 10, 17-38.	2.2	8
699	Development of nanoelectrospray high resolution isotope dilution mass spectrometry for targeted quantitative analysis of urinary metabolites: application to population profiling and clinical studies. Analytical Methods, 2015, 7, 5122-5133.	2.7	8
700	Automatic Spectroscopic Data Categorization by Clustering Analysis (ASCLAN): A Data-Driven Approach for Distinguishing Discriminatory Metabolites for Phenotypic Subclasses. Analytical Chemistry, 2016, 88, 5670-5679.	6.5	8
701	A validated UPLC-MS/MS assay for the quantification of amino acids and biogenic amines in rat urine. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2019, 1106-1107, 50-57.	2.3	8
702	Development and validation of a high performance liquid chromatography-tandem mass spectrometry method for the absolute analysis of 17 $\pm$ D-amino acids in cooked meals. Journal of Chromatography A, 2020, 1611, 460598.	3.7	8

#	ARTICLE	IF	CITATIONS
703	Higher premorbid serum testosterone predicts COVID-19-related mortality risk in men. <i>European Journal of Endocrinology</i> , 2022, 187, 159-170.	3.7	8
704	A study of the metabolism of dimethylformamide in the rat by high resolution proton NMR spectroscopy. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1989, 7, 499-505.	2.8	7
705	Comparison of in vivo <sup>1</sup> H MRS of human brain tumours with <sup>1</sup> H HR-MAS spectroscopy of intact biopsy samples in vitro. <i>Magnetic Resonance Materials in Physics, Biology, and Medicine</i> , 1999, 8, 121-128.	2.0	7
706	Rapid multi-component detection of fluorinated drug metabolites in whole urine from a <sup>19</sup> F cassette™ dose study using high resolution <sup>19</sup> F NMR spectroscopy. <i>Analytical Communications</i> , 1999, 36, 259-261.	2.2	7
707	2.7.5. HPLC/NMR and related hyphenated NMR methods. <i>Progress in Pharmaceutical and Biomedical Analysis</i> , 2000, 4, 299-322.	0.1	7
708	Application of <sup>1</sup> H- and <sup>19</sup> F-NMR spectroscopy in the investigation of the urinary and biliary excretion of 3,5-, 2,4-ditrifluoromethylbenzoic and pentafluorobenzoic acids in rat. <i>Xenobiotica</i> , 2002, 32, 605-613.	1.1	7
709	<sup>19</sup> F NMR spectroscopic investigation into the absorption and metabolism of 3-trifluoromethylaniline in <i>Eisenia veneta</i> . <i>Ecotoxicology and Environmental Safety</i> , 2003, 54, 157-168.	6.0	7
710	Cellular acidosis in rodents exposed to cadmium is caused by adaptation of the tissue rather than an early effect of toxicity. <i>Comparative Biochemistry and Physiology Part D: Genomics and Proteomics</i> , 2007, 2, 316-321.	1.0	7
711	Translational utility of a hierarchical classification strategy in biomolecular data analytics. <i>Scientific Reports</i> , 2017, 7, 14981.	3.3	7
712	Network Mapping of Molecular Biomarkers Influencing Radiation Response in Rectal Cancer. <i>Clinical Colorectal Cancer</i> , 2019, 18, e210-e222.	2.3	7
713	A targeted ultra performance liquid chromatography <sup>19</sup> F Tandem mass spectrometric assay for tyrosine and metabolites in urine and plasma: Application to the effects of antibiotics on mice. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2021, 1164, 122511.	2.3	7
714	A Nuclear Magnetic Resonance Approach to Investigate the Biochemical and Molecular Effects of Nephrotoxins. , 1987, , 397-408.		7
715	Abstract 3977: iKnife: Rapid evaporative ionization mass spectrometry (REIMS) enables real-time chemical analysis of the mucosal lipidome for diagnostic and prognostic use in colorectal cancer. , 2016, , .		7
716	Comparative distributions of zinc, cadmium and mercury in the tissues of experimental mice. <i>Comparative Biochemistry and Physiology Part C: Comparative Pharmacology</i> , 1984, 77, 249-256.	0.2	6
717	APPLICATION OF HIGH RESOLUTION H-NMR SPECTROSCOPY TO THE DETECTION OF PENICILLAMINE AND ITS METABOLITES IN HUMAN URINE. <i>Drug Metabolism and Drug Interactions</i> , 1988, 6, 439-446.	0.3	6
718	<sup>1</sup> H NMR spectroscopic studies on the characterization of renal cell lines and identification of novel potential markers of in vitro nephrotoxicity. <i>Biomarkers</i> , 1996, 1, 35-43.	1.9	6
719	Quantitative Investigation of Probabilistic Spectral Processing Methods Using Simulated NMR Data. <i>Applied Spectroscopy</i> , 2001, 55, 1214-1224.	2.2	6
720	Detection of mono- and di-hexoses as metabolites of 4-bromoaniline using HPLC-TOF-MS/MS. <i>Xenobiotica</i> , 2003, 33, 855-869.	1.1	6

#	ARTICLE	IF	CITATIONS
721	Investigation of basic mobile phases with positive ESI LC-MS for metabonomics studies. <i>Bioanalysis</i> , 2012, 4, 2833-2842.	1.5	6
722	Surgical systems biology and personalized longitudinal phenotyping in critical care. <i>Personalized Medicine</i> , 2012, 9, 593-608.	1.5	6
723	The Modulation of Drug Efficacy and Toxicity by the Gut Microbiome. <i>Molecular and Integrative Toxicology</i> , 2015, , 323-341.	0.5	6
724	Systems toxicology: modelling biomarkers of glutathione homeostasis and paracetamol metabolism. <i>Drug Discovery Today: Technologies</i> , 2015, 15, 9-14.	4.0	6
725	Obesity and Cage Environment Modulate Metabolism in the Zucker Rat: A Multiple Biological Matrix Approach to Characterizing Metabolic Phenomena. <i>Journal of Proteome Research</i> , 2019, 18, 2160-2174.	3.7	6
726	Metabolic Phenotyping Using UPLC-MS and Rapid Microbore UPLC-IMS: Determination of the Effect of Different Dietary Regimes on the Urinary Metabolome of the Rat. <i>Chromatographia</i> , 2020, 83, 853-861.	1.3	6
727	Comparison of Maximum Quantum Filtered NMR Spectroscopy (MAXY NMR) and Other Two-Dimensional NMR Approaches for Resonance Assignment of Peptides. , 1996, 34, 865-872.		5
728	Investigation of water environments in a C18 bonded silica phase using <sup>1</sup> H magic angle spinning (MAS) nuclear magnetic resonance (NMR) spectroscopy. <i>Analyst</i> , The, 2001, 126, 548-550.	3.5	5
729	Biomedical and Pharmaceutical Applications of HPLC-NMR and HPLC-NMR-MS. , 0, , 45-87.		5
730	Characterisation of the vaginal microbiome in cervical intraepithelial neoplasia. <i>Lancet</i> , The, 2016, 387, S75.	13.7	5
731	Probing the Reactivity of the Zinc and Cadmium Ions Bound to Rabbit Liver Metallothioneins with EDTA. <i>Exs</i> , 1987, 52, 191-201.	1.4	5
732	Application of inductively coupled plasma mass spectrometry and high-performance liquid chromatography with parallel electrospray mass spectrometry to the investigation of the disposition and metabolic fate of 2-, 3- and 4-iodobenzoic acids in the rat. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2004, 809, 279-285.	2.3	5
733	Biofluids Studied By NMR. , 1999, , 98-116.		4
734	UPLC-MS, HPLC-radiometric, and NMR-spectroscopic studies on the metabolic fate of 3-fluoro-[U- <sup>14</sup> C]-aniline in the bile-cannulated rat. <i>Xenobiotica</i> , 2010, 40, 510-523.	1.1	4
735	Initial non-repetitive complexity of infinite words. <i>Discrete Applied Mathematics</i> , 2016, 208, 114-122.	0.9	4
736	Studies of the biochemical toxicology of uranyl nitrate in the rat. <i>Archives of Toxicology</i> , 1994, 68, 43.	4.2	4
737	Spatially resolved profiling of colorectal cancer lipid biochemistry via DESI imaging mass spectrometry to reveal morphology-dependent alterations in fatty acid metabolism.. <i>Journal of Clinical Oncology</i> , 2016, 34, e15104-e15104.	1.6	4
738	NMR Studies of Crab and Plaice Metallothioneins. <i>Environmental Health Perspectives</i> , 1986, 65, 157.	6.0	3



#	ARTICLE	IF	CITATIONS
739	Neuroendocrine Neoplasms: Identification of Novel Metabolic Circuits of Potential Diagnostic Utility. <i>Cancers</i> , 2021, 13, 374.	3.7	3
740	Proton MRS of human prostatic fluid: Correlations between citrate, spermine, and myo-inositol levels and changes with disease. <i>Prostate</i> , 1997, 30, 248-255.	2.3	3
741	Quantitative Structure-Toxicity Relationships for Chlorophenols to Bioluminescent <i>Lux</i> -Marked Bacteria Using Atom-Based Semi-Empirical Molecular-Orbital Descriptors. <i>SAR and QSAR in Environmental Research</i> , 1999, 10, 473-495.	2.2	2
742	The metabolism and excretion of [14C] 2- and 4-chlorobenzoic acids in the rat. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2000, 22, 1023-1028.	2.8	2
743	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.	2.6	2
744	Biomedical applications of directly-coupled chromatography-nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry (MS). <i>Handbook of Analytical Separations</i> , 2003, , 293-329.	0.8	2
745	Metabolism of [14C]-5-chloro-1,3-benzodioxol-4-amine in male Wistar-derived rats following intraperitoneal administration. <i>Xenobiotica</i> , 2007, 37, 44-58.	1.1	2
746	Response to Comment on "Optimized Preprocessing of Ultra-Performance Liquid Chromatography/Mass Spectrometry Urinary Metabolic Profiles for Improved Information Recovery". <i>Analytical Chemistry</i> , 2011, 83, 9721-9722.	6.5	2
747	The metabolic fate and effects of 2-Bromophenol in male Sprague-Dawley rats. <i>Xenobiotica</i> , 2019, 49, 1352-1359.	1.1	2
748	Dietary fibre to reduce colon cancer risk in Alaska Native people: the Alaska FIRST randomised clinical trial protocol. <i>BMJ Open</i> , 2021, 11, e047162.	1.9	2
749	Metabonomics: Metabolic processes studied by NMR spectroscopy of biofluids. , 0, .		2
750	Modeling People and Populations. , 2016, , 333-367.		2
751	NMR and QSAR studies on the transacylation reactivity of model 1 <sup>2</sup> - O -acyl glucuronides. I: Design, synthesis and degradation rate measurement. <i>Xenobiotica</i> , 2004, 34, 73-85.	1.1	2
752	Unmet Medical Needs. , 2016, , 1-15.		2
753	Asymptomatic 5-oxoprolinuria detected by proton magnetic resonance spectroscopy. <i>Clinical Chemistry</i> , 1993, 39, 1341.	3.2	2
754	Medium-Sulfur Coal and Fly Ash Resistivity. <i>Japca</i> , 1988, 38, 209-216.	0.3	1
755	Revised method of proton NMR urinalysis for detecting inborn errors of metabolism: a critique.. <i>Clinical Chemistry</i> , 1988, 34, 213-215.	3.2	1
756	An NMR study of the metabolic fate of 2-, 3- and 4-fluorobenzyl alcohols in the rat. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2003, 32, 133-140.	2.8	1

#	ARTICLE	IF	CITATIONS
757	Metabonomics. , 2005, , 41-46.		1
758	NMR-based Metabonomics Techniques and Applications. , 2008, , 1377-1385.		1
759	1869: Nuclear Magnetic Resonance Based Metabonomic Investigation of Semen, Urine and Plasma Metabolite Profiles in Healthy Volunteers and Men with Spinal Cord Injury. Journal of Urology, 2007, 177, 620-620.	0.4	1
760	The Metabolic Window into Systems Biology. Journal of Proteome Research, 2007, 6, 433-433.	3.7	1
761	Method Development of Efficient Protein Extraction in Bone Tissue for Proteome Analysis]. Proteome Res.2007,6, 2287~2294.. Journal of Proteome Research, 2007, 6, 4528-4528.	3.7	1
762	Milk modulates the microbiota. Nature Medicine, 2012, 18, 1186-1187.	30.7	1
763	Phenotyping the Patient Journey. , 2016, , 49-74.		1
764	Pharmacometabonomics and Predictive Metabonomics. , 2016, , 137-165.		1
765	Correction to 2-Furoylglycine as a Candidate Biomarker of Coffee Consumption. Journal of Agricultural and Food Chemistry, 2016, 64, 8958-8958.	5.2	1
766	The Frobenius problem for the shuffle operation. Semigroup Forum, 2018, 96, 160-177.	0.6	1
767	Strategy for improved characterization of human metabolic phenotypes using a COmbined Multi-block Principal components Analysis with Statistical Spectroscopy (COMPASS). Bioinformatics, 2021, 36, 5229-5236.	4.1	1
768	High Resolution Nuclear Magnetic Resonance Spectroscopy in Clinical Chemistry and Disease Diagnosis. , 1989, , 9-26.		1
769	Abstract 4974: Prospective study of untargeted urinary metabolomics and risk of lung cancer among female never-smokers in Shanghai, China. , 2018, , .		1
770	Novel data processing and image co-registration algorithm for region-specific lipid profiling in colorectal cancer tissue using DESI imaging mass spectrometry.. Journal of Clinical Oncology, 2013, 31, e14620-e14620.	1.6	1
771	Global Systems Biology Through Integration of Omics•Results. , 2007, , 533-555.		1
772	Abstract 5269: Discovery and validation of plasma acylcarnitines for the early diagnosis of hepatocellular carcinoma. , 2019, , .		1
773	Revised method of proton NMR urinalysis for detecting inborn errors of metabolism: a critique. Clinical Chemistry, 1988, 34, 213-5.	3.2	1
774	NMR and QSAR studies on the transacylation reactivity of model 1beta-O-acyl glucuronides. I: design, synthesis and degradation rate measurement. Xenobiotica, 2004, 34, 73-85.	1.1	1

#	ARTICLE	IF	CITATIONS
775	Biomedical and pharmaceutical chemistry. Analytical Proceedings, 1991, 28, 177.	0.4	0
776	Measurement of longitudinal relaxation times in crowded $^1\text{H}$ NMR spectra using one- and two-dimensional maximum quantum (MAXY) NMR spectroscopy. Molecular Physics, 2001, 99, 1701-1707.	1.7	0
777	Metabolism and Metabolites: Putting Proteomes into Perspective. Journal of Proteome Research, 2005, 4, 13-13.	3.7	0
778	Exploring the Contribution of Metabolic Profiling to Epidemiological Studies. , 0, , 167-180.		0
779	The Development of a Metabonomic-Based Drug Safety Testing Paradigm. , 0, , 309-343.		0
780	Statistical Tools for Molecular Covariance Spectroscopy. , 2017, , 243-249.		0
781	Conception, Implementation and Operation of Large-Scale Metabolic Phenotyping Centres: Phenome Centres. , 2019, , 385-405.		0
782	Metabolic Phenotyping: History, Status, and Prospects. , 2019, , 571-583.		0
783	Metabonomics as a Tool for Understanding Lipid Metabolism. , 2004, , 405-422.		0
784	Metabonomics and Its Role in Disease Diagnosis. , 2004, , 797-802.		0
785	An Overview of Metabonomics. , 2005, , 1-26.		0
786	The Application of High Resolution Proton NMR Spectroscopy to the Detection of Drug Metabolites in Biological Samples. , 1986, , 321-335.		0
787	Proton Nuclear Magnetic Spectroscopy: A Novel Method for the Study of Solid Phase Extraction. , 1994, , 37-52.		0
788	Future Visions for Clinical Metabolic Phenotyping. , 2016, , 369-388.		0
789	Abstract 839: Network-driven analytics of published tissue-based biomarkers to predict response to neoadjuvant therapy in rectal cancer. , 2017, , .		0
790	Application of novel solid phase extraction-NMR protocols for metabolic profiling of human urine. Faraday Discussions, 2019, 218, 395-416.	3.2	0
791	Metabolic Modeling in Health and Disease. Journal of Proteome Research, 2022, 21, 559-559.	3.7	0