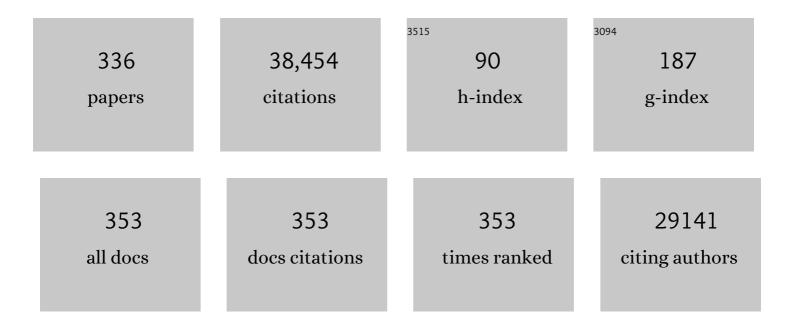
List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Proposed minimum reporting standards for chemical analysis. Metabolomics, 2007, 3, 211-221.	1.4	3,589
2	Metabolic profiling, metabolomic and metabonomic procedures for NMR spectroscopy of urine, plasma, serum and tissue extracts. Nature Protocols, 2007, 2, 2692-2703.	5.5	1,830
3	Metabonomics: a platform for studying drug toxicity and gene function. Nature Reviews Drug Discovery, 2002, 1, 153-161.	21.5	1,739
4	Metabonomics. Nature, 2008, 455, 1054-1056.	13.7	1,660
5	750 MHz 1H and 1H-13C NMR Spectroscopy of Human Blood Plasma. Analytical Chemistry, 1995, 67, 793-811.	3.2	972
6	Metabolic profiling reveals a contribution of gut microbiota to fatty liver phenotype in insulin-resistant mice. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 12511-12516.	3.3	948
7	Statistical Total Correlation Spectroscopy:Â An Exploratory Approach for Latent Biomarker Identification from Metabolic1H NMR Data Sets. Analytical Chemistry, 2005, 77, 1282-1289.	3.2	833
8	Pharmaco-metabonomic phenotyping and personalized drug treatment. Nature, 2006, 440, 1073-1077.	13.7	787
9	Pharmacometabonomic identification of a significant host-microbiome metabolic interaction affecting human drug metabolism. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 14728-14733.	3.3	665
10	Evaluation of the Orthogonal Projection on Latent Structure Model Limitations Caused by Chemical Shift Variability and Improved Visualization of Biomarker Changes in1H NMR Spectroscopic Metabonomic Studies. Analytical Chemistry, 2005, 77, 517-526.	3.2	553
11	Improved WATERGATE Pulse Sequences for Solvent Suppression in NMR Spectroscopy. Journal of Magnetic Resonance, 1998, 132, 125-129.	1.2	518
12	Metabolic phenotyping in clinical and surgical environments. Nature, 2012, 491, 384-392.	13.7	450
13	Scaling and Normalization Effects in NMR Spectroscopic Metabonomic Data Sets. Analytical Chemistry, 2006, 78, 2262-2267.	3.2	438
14	Metabonomics technologies and their applications in physiological monitoring, drug safety assessment and disease diagnosis. Biomarkers, 2004, 9, 1-31.	0.9	425
15	NMR-based metabonomic approaches for evaluating physiological influences on biofluid composition. NMR in Biomedicine, 2005, 18, 143-162.	1.6	425
16	A topâ€down systems biology view of microbiomeâ€mammalian metabolic interactions in a mouse model. Molecular Systems Biology, 2007, 3, 112.	3.2	420
17	Precision High-Throughput Proton NMR Spectroscopy of Human Urine, Serum, and Plasma for Large-Scale Metabolic Phenotyping. Analytical Chemistry, 2014, 86, 9887-9894.	3.2	419
18	Metabonomics: Metabolic processes studied by NMR spectroscopy of biofluids. Concepts in Magnetic Resonance, 2000, 12, 289-320.	1.3	401

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19	The metabolomics standards initiative (MSI). Metabolomics, 2007, 3, 175-178.	1.4	396
20	Probiotic modulation of symbiotic gut microbial–host metabolic interactions in a humanized microbiome mouse model. Molecular Systems Biology, 2008, 4, 157.	3.2	392
21	Pattern recognition methods and applications in biomedical magnetic resonance. Progress in Nuclear Magnetic Resonance Spectroscopy, 2001, 39, 1-40.	3.9	384
22	Contemporary issues in toxicology the role of metabonomics in toxicology and its evaluation by the COMET project. Toxicology and Applied Pharmacology, 2003, 187, 137-146.	1.3	374
23	High-resolution magic-angle-spinning NMR spectroscopy for metabolic profiling of intact tissues. Nature Protocols, 2010, 5, 1019-1032.	5.5	355
24	The challenges of modeling mammalian biocomplexity. Nature Biotechnology, 2004, 22, 1268-1274.	9.4	351
25	Colonization-Induced Host-Gut Microbial Metabolic Interaction. MBio, 2011, 2, e00271-10.	1.8	342
26	Susceptibility of Human Metabolic Phenotypes to Dietary Modulation. Journal of Proteome Research, 2006, 5, 2780-2788.	1.8	337
27	Assessment of Analytical Reproducibility of1H NMR Spectroscopy Based Metabonomics for Large-Scale Epidemiological Research:Â the INTERMAP Study. Analytical Chemistry, 2006, 78, 2199-2208.	3.2	332
28	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.	3.2	330
29	The Metabolomics Standards Initiative. Nature Biotechnology, 2007, 25, 846-848.	9.4	328
30	NMR Spectroscopy of Biofluids. Annual Reports on NMR Spectroscopy, 1999, 38, 1-88.	0.7	314
31	Recursive Segment-Wise Peak Alignment of Biological <sup>1</sup> H NMR Spectra for Improved Metabolic Biomarker Recovery. Analytical Chemistry, 2009, 81, 56-66.	3.2	303
32	NMR-Based Metabolic Profiling and Metabonomic Approaches to Problems in Molecular Toxicology. Chemical Research in Toxicology, 2008, 21, 9-27.	1.7	289
33	Chemometric Models for Toxicity Classification Based on NMR Spectra of Biofluids. Chemical Research in Toxicology, 2000, 13, 471-478.	1.7	277
34	The Consortium for Metabonomic Toxicology (COMET): aims, activities and achievements. Pharmacogenomics, 2005, 6, 691-699.	0.6	277
35	Urinary Metabolic Phenotyping Differentiates Children with Autism from Their Unaffected Siblings and Age-Matched Controls. Journal of Proteome Research, 2010, 9, 2996-3004.	1.8	277
36	Spectroscopic and Statistical Techniques for Information Recovery in Metabonomics and Metabolomics. Annual Review of Analytical Chemistry, 2008, 1, 45-69.	2.8	270

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37	Analytical Reproducibility in1H NMR-Based Metabonomic Urinalysis. Chemical Research in Toxicology, 2002, 15, 1380-1386.	1.7	261
38	Summary recommendations for standardization and reporting of metabolic analyses. Nature Biotechnology, 2005, 23, 833-838.	9.4	261
39	Metabonomics in pharmaceutical R & D. FEBS Journal, 2007, 274, 1140-1151.	2.2	258
40	Metabonomics Techniques and Applications to Pharmaceutical Research & Development. Pharmaceutical Research, 2006, 23, 1075-1088.	1.7	256
41	An Integrated Metabonomic Investigation of Acetaminophen Toxicity in the Mouse Using NMR Spectroscopy. Chemical Research in Toxicology, 2003, 16, 295-303.	1.7	245
42	Optimized Preprocessing of Ultra-Performance Liquid Chromatography/Mass Spectrometry Urinary Metabolic Profiles for Improved Information Recovery. Analytical Chemistry, 2011, 83, 5864-5872.	3.2	240
43	Use of relaxation-edited one-dimensional and two dimensional nuclear magnetic resonance spectroscopy to improve detection of small metabolites in blood plasma. Analytical Biochemistry, 2004, 325, 260-272.	1.1	212
44	Cryogenic Probe 13C NMR Spectroscopy of Urine for Metabonomic Studies. Analytical Chemistry, 2002, 74, 4588-4593.	3.2	200
45	Peer Reviewed: So What's the Deal with Metabonomics?. Analytical Chemistry, 2003, 75, 384 A-391 A.	3.2	189
46	Metabonomic Investigations into Hydrazine Toxicity in the Rat. Chemical Research in Toxicology, 2001, 14, 975-987.	1.7	179
47	Directly coupled HPLC–NMR and HPLC–NMR–MS in pharmaceutical research and development. Biomedical Applications, 2000, 748, 233-258.	1.7	177
48	Species Variation in the Fecal Metabolome Gives Insight into Differential Gastrointestinal Function. Journal of Proteome Research, 2008, 7, 352-360.	1.8	170
49	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.	3.2	169
50	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.	3.2	165
51	Improved analysis of multivariate data by variable stability scaling: application to NMR-based metabolic profiling. Analytica Chimica Acta, 2003, 490, 265-276.	2.6	164
52	Prediction and Classification of Drug Toxicity Using Probabilistic Modeling of Temporal Metabolic Data:Â The Consortium on Metabonomic Toxicology Screening Approach. Journal of Proteome Research, 2007, 6, 4407-4422.	1.8	164
53	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.	1.4	163
54	Metabonomics and its role in drug development and disease diagnosis. Expert Review of Molecular Diagnostics, 2004, 4, 189-199.	1.5	161

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55	Human metabolic profiles are stably controlled by genetic and environmental variation. Molecular Systems Biology, 2011, 7, 525.	3.2	158
56	Human Metabolic Phenotypes Link Directly to Specific Dietary Preferences in Healthy Individuals. Journal of Proteome Research, 2007, 6, 4469-4477.	1.8	156
57	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.	1.4	152
58	Panorganismal Gut Microbiomeâ^'Host Metabolic Crosstalk. Journal of Proteome Research, 2009, 8, 2090-2105.	1.8	151
59	High-Resolution Diffusion and Relaxation Edited One- and Two-Dimensional1H NMR Spectroscopy of Biological Fluids. Analytical Chemistry, 1996, 68, 3370-3376.	3.2	145
60	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.	1.1	144
61	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.	1.8	143
62	Geometric Trajectory Analysis of Metabolic Responses To Toxicity Can Define Treatment Specific Profiles. Chemical Research in Toxicology, 2004, 17, 579-587.	1.7	143
63	NMR-based metabonomic toxicity classification: hierarchical cluster analysis and k-nearest-neighbour approaches. Analytica Chimica Acta, 2003, 490, 3-15.	2.6	142
64	The Comparison of Plasma Deproteinization Methods for the Detection of Low-Molecular-Weight Metabolites by 1H Nuclear Magnetic Resonance Spectroscopy. Analytical Biochemistry, 2002, 304, 220-230.	1.1	140
65	Direct coupling of chromatographic separations to NMR spectroscopy. Progress in Nuclear Magnetic Resonance Spectroscopy, 1996, 29, 1-49.	3.9	137
66	Pharmacometabonomics as an effector for personalized medicine. Pharmacogenomics, 2011, 12, 103-111.	0.6	136
67	HILIC-UPLC-MS for Exploratory Urinary Metabolic Profiling in Toxicological Studies. Analytical Chemistry, 2011, 83, 382-390.	3.2	135
68	Biochemical classification of kidney carcinoma biopsy samples using magic-angle-spinning 1H nuclear magnetic resonance spectroscopy. Journal of Pharmaceutical and Biomedical Analysis, 1998, 17, 125-132.	1.4	133
69	A Genome-Wide Metabolic QTL Analysis in Europeans Implicates Two Loci Shaped by Recent Positive Selection. PLoS Genetics, 2011, 7, e1002270.	1.5	132
70	Environmental Metabonomics: Applying Combination Biomarker Analysis in Earthworms at a Metal Contaminated Site. Ecotoxicology, 2004, 13, 797-806.	1.1	128
71	Comparative metabonomics of differential hydrazine toxicity in the rat and mouse. Toxicology and Applied Pharmacology, 2005, 204, 135-151.	1.3	125
72	Analytical technologies for metabonomics and metabolomics, and multi-omic information recovery. TrAC - Trends in Analytical Chemistry, 2008, 27, 194-204.	5.8	125

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73	Robust Data Processing and Normalization Strategy for MALDI Mass Spectrometric Imaging. Analytical Chemistry, 2012, 84, 1310-1319.	3.2	123
74	NMR spectroscopy as a novel approach to the monitoring of renal transplant function. Kidney International, 1993, 43, 234-245.	2.6	118
75	Detection of Urinary Drug Metabolite (Xenometabolome) Signatures in Molecular Epidemiology Studies via Statistical Total Correlation (NMR) Spectroscopy. Analytical Chemistry, 2007, 79, 2629-2640.	3.2	118
76	Acyl Glucuronides:  Biological Activity, Chemical Reactivity, and Chemical Synthesis. Journal of Medicinal Chemistry, 2006, 49, 6931-6945.	2.9	116
77	High resolution magic angle spinning 1H nuclear magnetic resonance analysis of intact prostatic hyperplastic and tumour tissues. Analytical Communications, 1998, 35, 113-115.	2.2	114
78	Stability and Robustness of Human Metabolic Phenotypes in Response to Sequential Food Challenges. Journal of Proteome Research, 2012, 11, 643-655.	1.8	113
79	Development and Application of Ultra-Performance Liquid Chromatography-TOF MS for Precision Large Scale Urinary Metabolic Phenotyping. Analytical Chemistry, 2016, 88, 9004-9013.	3.2	113
80	Metabonomic assessment of toxicity of 4â€fluoroaniline, 3,5â€difluoroaniline and 2â€fluoroâ€4â€methylaniline to the earthworm <i>Eisenia veneta</i> (rosa): Identification of new endogenous biomarkers. Environmental Toxicology and Chemistry, 2002, 21, 1966-1972.	2.2	110
81	Metabonomic Studies on the Physiological Effects of Acute and Chronic Psychological Stress in Spragueâ^'Dawley Rats. Journal of Proteome Research, 2007, 6, 2080-2093.	1.8	109
82	High-resolution magic angle spinning NMR spectroscopy: Application to biomedical studies. Progress in Nuclear Magnetic Resonance Spectroscopy, 2009, 55, 79-100.	3.9	108
83	Serum metabolic signatures of coronary and carotid atherosclerosis and subsequent cardiovascular disease. European Heart Journal, 2019, 40, 2883-2896.	1.0	107
84	Directly Coupled HPLC-NMR and Its Application to Drug Metabolism. Drug Metabolism Reviews, 1997, 29, 705-746.	1.5	104
85	Identification of Human Urinary Biomarkers of Cruciferous Vegetable Consumption by Metabonomic Profiling. Journal of Proteome Research, 2011, 10, 4513-4521.	1.8	104
86	Metabolic Assessment of Human Liver Transplants from Biopsy Samples at the Donor and Recipient Stages Using High-Resolution Magic Angle Spinning1H NMR Spectroscopy. Analytical Chemistry, 2005, 77, 5570-5578.	3.2	102
87	A metabolic system-wide characterisation of the pig: a model for human physiology. Molecular BioSystems, 2011, 7, 2577.	2.9	101
88	Evaluation of Full-Resolution <i>J</i> -Resolved <sup>1</sup> H NMR Projections of Biofluids for Metabonomics Information Retrieval and Biomarker Identification. Analytical Chemistry, 2010, 82, 1811-1821.	3.2	96
89	Distinction between normal and renal cell carcinoma kidney cortical biopsy samples using pattern recognition of1H magic angle spinning (MAS) NMR spectra. NMR in Biomedicine, 2000, 13, 64-71.	1.6	94
90	UPLC-MS metabolic profiling of second trimester amniotic fluid and maternal urine and comparison with NMR spectral profiling for the identification of pregnancy disorder biomarkers. Molecular BioSystems, 2012, 8, 1243.	2.9	94

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91	Hyperspectral Visualization of Mass Spectrometry Imaging Data. Analytical Chemistry, 2013, 85, 1415-1423.	3.2	93
92	An Integrated Metabonomic Approach To Describe Temporal Metabolic Disregulation Induced in the Rat by the Model Hepatotoxin Allyl Formate. Journal of Proteome Research, 2006, 5, 2675-2684.	1.8	90
93	Earthworm species of the genus Eisenia can be phenotypically differentiated by metabolic profiling. FEBS Letters, 2002, 521, 115-120.	1.3	89
94	Ultra Performance Liquid Chromatography-Mass Spectrometry Profiling of Bile Acid Metabolites in Biofluids: Application to Experimental Toxicology Studies. Analytical Chemistry, 2010, 82, 5282-5289.	3.2	89
95	Automatic alignment of individual peaks in large high-resolution spectral data sets. Journal of Magnetic Resonance, 2004, 170, 329-335.	1.2	88
96	Effects of ProbioticLactobacillusParacaseiTreatment on the Host Gut Tissue Metabolic Profiles ProbedviaMagic-Angle-Spinning NMR Spectroscopy. Journal of Proteome Research, 2007, 6, 1471-1481.	1.8	88
97	<sup>1</sup> H NMR Spectroscopy-Based Interventional Metabolic Phenotyping: A Cohort Study of Rheumatoid Arthritis Patients. Journal of Proteome Research, 2010, 9, 4545-4553.	1.8	88
98	Statistical Correlation and Projection Methods for Improved Information Recovery from Diffusion-Edited NMR Spectra of Biological Samples. Analytical Chemistry, 2007, 79, 5682-5689.	3.2	87
99	Directly Coupled 800 MHz HPLCâ <sup>~</sup> 'NMR Spectroscopy of Urine and Its Application to the Identification of the Major Phase II Metabolites of Tolfenamic Acid. Analytical Chemistry, 1997, 69, 607-612.	3.2	86
100	Topâ€down systems biology integration of conditional prebiotic modulated transgenomic interactions in a humanized microbiome mouse model. Molecular Systems Biology, 2008, 4, 205.	3.2	86
101	Incomplete Systemic Recovery and Metabolic Phenoreversion in Post-Acute-Phase Nonhospitalized COVID-19 Patients: Implications for Assessment of Post-Acute COVID-19 Syndrome. Journal of Proteome Research, 2021, 20, 3315-3329.	1.8	85
102	600 MHz 1H-NMR spectroscopy of human cerebrospinal fluid: Effects of sample manipulation and assignment of resonances. Journal of Pharmaceutical and Biomedical Analysis, 1993, 11, 651-664.	1.4	81
103	Measurement of Biomolecular Diffusion Coefficients in Blood Plasma Using Two-Dimensional 1Hâ^'1H Diffusion-Edited Total-Correlation NMR Spectroscopy. Analytical Chemistry, 1997, 69, 1504-1509.	3.2	81
104	Metabolomics Standards Workshop and the development of international standards for reporting metabolomics experimental results. Briefings in Bioinformatics, 2006, 7, 159-165.	3.2	81
105	Statistical Spectroscopic Tools for Biomarker Discovery and Systems Medicine. Analytical Chemistry, 2013, 85, 5297-5303.	3.2	77
106	Toxicity classification from metabonomic data using a density superposition approach: â€~CLOUDS'. Analytica Chimica Acta, 2003, 490, 109-122.	2.6	76
107	Transgenomic Metabolic Interactions in a Mouse Disease Model:Â Interactions ofTrichinellaspiralisInfection with DietaryLactobacillusparacaseiSupplementation. Journal of Proteome Research, 2006, 5, 2185-2193.	1.8	76
108	Experimental Metabonomic Model of Dietary Variation and Stress Interactions. Journal of Proteome Research, 2006, 5, 1535-1542.	1.8	75

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109	NMR-Based Metabolic Profiling Identifies Biomarkers of Liver Regeneration Following Partial Hepatectomy in the Rat. Journal of Proteome Research, 2010, 9, 59-69.	1.8	75
110	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. Analytical Chemistry, 2012, 84, 10694-10701.	3.2	75
111	The emergent role of metabolic phenotyping in dynamic patient stratification. Expert Opinion on Drug Metabolism and Toxicology, 2014, 10, 915-919.	1.5	75
112	Topographical Variation in Metabolic Signatures of Human Gastrointestinal Biopsies Revealed by High-Resolution Magic-Angle Spinning <sup>1</sup> H NMR Spectroscopy. Journal of Proteome Research, 2007, 6, 3944-3951.	1.8	72
113	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
114	Identifying unknown metabolites using NMR-based metabolic profiling techniques. Nature Protocols, 2020, 15, 2538-2567.	5.5	69
115	Classification of toxin-induced changes in 1H NMR spectra of urine using an artificial neural network. Journal of Pharmaceutical and Biomedical Analysis, 1995, 13, 205-211.	1.4	65
116	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.	1.8	64
117	Magic Angle Spinning Proton Nuclear Magnetic Resonance Spectroscopic Analysis of Intact Kidney Tissue Samples. Analytical Communications, 1997, 34, 107-109.	2.2	63
118	Detection ofin vivo biomarkers of phospholipidosis using NMR-based metabonomic approaches. Magnetic Resonance in Chemistry, 2001, 39, 559-565.	1.1	62
119	Topographical Variation in Murine Intestinal Metabolic Profiles in Relation to Microbiome Speciation and Functional Ecological Activity. Journal of Proteome Research, 2009, 8, 3464-3474.	1.8	62
120	NMR-Based Metabonomic Studies on the Biochemical Effects of Epicatechin in the Rat. Journal of Agricultural and Food Chemistry, 2003, 51, 4139-4145.	2.4	61
121	Biochemical Characterization of Rat Intestine Development Using High-Resolution Magic-Angle-Spinning1H NMR Spectroscopy and Multivariate Data Analysis. Journal of Proteome Research, 2005, 4, 1324-1329.	1.8	61
122	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.	1.8	61
123	High performance liquid chromatography coupled to nuclear magnetic resonance spectroscopy and mass spectrometry applied to plant products: Identification of ecdysteroids fromSilene otites. Chromatographia, 1999, 49, 374-378.	0.7	59
124	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.	1.4	59
125	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.	1.7	59
126	An hypothesis for a mechanism underlying hepatotoxin-induced hypercreatinuria. Archives of Toxicology, 2003, 77, 208-217.	1.9	59

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127	Omics and its potential impact on R&D and regulation of complex herbal products. Journal of Ethnopharmacology, 2012, 140, 587-593.	2.0	59
128	Heteronuclear <sup>1</sup> Hâ~' <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.	3.2	58
129	Robust Algorithms for Automated Chemical Shift Calibration of 1D 1H NMR Spectra of Blood Serum. Analytical Chemistry, 2008, 80, 7158-7162.	3.2	58
130	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.	1.8	57
131	Longitudinal pharmacometabonomics for predicting patient responses to therapy: drug metabolism, toxicity and efficacy. Expert Opinion on Drug Metabolism and Toxicology, 2012, 8, 135-139.	1.5	57
132	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
133	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. Analytical Chemistry, 2008, 80, 7354-7362.	3.2	56
134	Genetic algorithms for simultaneous variable and sample selection in metabonomics. Bioinformatics, 2009, 25, 112-118.	1.8	56
135	Metabonomics: systems biology in pharmaceutical research and development. Current Opinion in Molecular Therapeutics, 2004, 6, 265-72.	2.8	56
136	Use of1H NMR-determined diffusion coefficients to characterize lipoprotein fractions in human blood plasma. Magnetic Resonance in Chemistry, 2002, 40, S83-S88.	1.1	55
137	Temporal Metabonomic Modeling of <scp>l</scp> -Arginine-Induced Exocrine Pancreatitis. Journal of Proteome Research, 2008, 7, 4435-4445.	1.8	55
138	Characterisation of impurities in bulk drug batches of fluticasone propionate using directly coupled HPLC–NMR spectroscopy and HPLC–MS. Journal of Pharmaceutical and Biomedical Analysis, 1997, 16, 697-705.	1.4	53
139	Directly coupled CZE-NMR and CEC-NMR spectroscopy for metabolite analysis: paracetamol metabolites in human urine. Analyst, The, 1998, 123, 2835-2837.	1.7	53
140	Heteronuclear <sup>19</sup> Fâ^' <sup>1</sup> H Statistical Total Correlation Spectroscopy as a Tool in Drug Metabolism:  Study of Flucloxacillin Biotransformation. Analytical Chemistry, 2008, 80, 1073-1079.	3.2	53
141	Identification of metabolites in human hepatic bile using 800 MHz 1H NMR spectroscopy , HPLC-NMR/MS and UPLC-MS. Molecular BioSystems, 2009, 5, 180-190.	2.9	53
142	NMR spectroscopy of human post mortem cerebrospinal fluid: Distinction of Alzheimer's disease from control using pattern recognition and statistics. NMR in Biomedicine, 1993, 6, 163-167.	1.6	52
143	On-flow identification of metabolites of paracetamol from human urine using directly coupled CZE–NMR and CEC–NMR spectroscopy. Analytical Communications, 1998, 35, 213-215.	2.2	52
144	A metabonomic investigation of hepatotoxicity using diffusion-edited 1H NMR spectroscopy of blood serum. Analyst, The, 2003, 128, 814.	1.7	52

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145	Statistical Search Space Reduction and Two-Dimensional Data Display Approaches for UPLCâ^'MS in Biomarker Discovery and Pathway Analysis. Analytical Chemistry, 2006, 78, 4398-4408.	3.2	52
146	Data-Driven Approach for Metabolite Relationship Recovery in Biological <sup>1</sup> H NMR Data Sets Using Iterative Statistical Total Correlation Spectroscopy. Analytical Chemistry, 2011, 83, 2075-2082.	3.2	52
147	Magic Angle Spinning NMR and <sup>1</sup> Hâ^' <sup>31</sup> P Heteronuclear Statistical Total Correlation Spectroscopy of Intact Human Gut Biopsies. Analytical Chemistry, 2008, 80, 1058-1066.	3.2	51
148	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-[13C]-acetanilide in Rat Urine. Analytical Chemistry, 2001, 73, 1491-1494.	3.2	50
149	Studies of the biochemical toxicology of uranyl nitrate in the rat. Archives of Toxicology, 1994, 68, 43-53.	1.9	48
150	Identification of the Positional Isomers of 2-Fluorobenzoic acid 1-O-Acyl Glucuronide by Directly Coupled HPLC-NMR. Analytical Chemistry, 1995, 67, 3401-3404.	3.2	48
151	Analysis of Drug–Protein Binding Using Nuclear Magnetic Resonance Based Molecular Diffusion Measurements. Analytical Communications, 1997, 34, 225-228.	2.2	46
152	Integrated Analytical and Statistical Two-Dimensional Spectroscopy Strategy for Metabolite Identification: Application to Dietary Biomarkers. Analytical Chemistry, 2017, 89, 3300-3309.	3.2	46
153	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. Analytical Chemistry, 1995, 67, 4441-4445.	3.2	45
154	NMR Spectroscopic Studies on the in Vitro Acyl Glucuronide Migration Kinetics of Ibuprofen ((±)-( <i>R</i> , <i>S</i> )-2-(4-Isobutylphenyl) Propanoic Acid), Its Metabolites, and Analogues. Analytical Chemistry, 2007, 79, 8720-8727.	3.2	45
155	Quantitative structure-metabolism relationships for substituted benzoic acids in the rat. Biochemical Pharmacology, 1992, 44, 1935-1946.	2.0	44
156	Application of directly coupled LC–NMR–MS to the structural elucidation of metabolites of the HIV-1 reverse-transcriptase inhibitor BW935U83. Biomedical Applications, 2000, 748, 269-279.	1.7	44
157	A Rapid and Facile Method for the Dereplication of Purified Natural Products. Journal of Natural Products, 2001, 64, 1541-1544.	1.5	44
158	Hepatotoxin-induced hypercreatinaemia and hypercreatinuria: their relationship to one another, to liver damage and to weakened nutritional status. Archives of Toxicology, 2004, 78, 86-96.	1.9	44
159	Intra- and Interlaboratory Reproducibility of Ultra Performance Liquid Chromatography–Time-of-Flight Mass Spectrometry for Urinary Metabolic Profiling. Analytical Chemistry, 2012, 84, 2424-2432.	3.2	44
160	Diffusion and Relaxation Edited Proton NMR Spectroscopy of Plasma Reveals a High-Fidelity Supramolecular Biomarker Signature of SARS-CoV-2 Infection. Analytical Chemistry, 2021, 93, 3976-3986.	3.2	43
161	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. Analyst, The, 2000, 125, 235-236.	1.7	42
162	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. Archives of Toxicology, 1992, 66, 525-537.	1.9	41

#	Article	IF	CITATIONS
163	Measurement of Internal Acyl Migration Reaction Kinetics Using Directly Coupled HPLCâ`'NMR:Â Application for the Positional Isomers of Synthetic (2-Fluorobenzoyl)-d-glucopyranuronic Acid. Analytical Chemistry, 1996, 68, 2564-2572.	3.2	41
164	The urinary proteome and metabonome differ from normal in adults with mitochondrial disease. Kidney International, 2015, 87, 610-622.	2.6	41
165	750 MHz HPLCâ^'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. Analytical Chemistry, 1996, 68, 106-110.	3.2	40
166	Direct observation of resolved intracellular and extracellular water signals in intact human red blood cells using1H MAS NMR spectroscopy. Magnetic Resonance in Medicine, 1997, 38, 334-336.	1.9	40
167	Mechanistic Aspects and Novel Biomarkers of Responder and Non-Responder Phenotypes in Galactosamine-Induced Hepatitis. Journal of Proteome Research, 2009, 8, 5175-5187.	1.8	39
168	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. Journal of Proteome Research, 2020, 19, 4428-4441.	1.8	39
169	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
170	Sample Classification Based on Bayesian Spectral Decomposition of Metabonomic NMR Data Sets. Analytical Chemistry, 2004, 76, 3666-3674.	3.2	38
171	Statistical Total Correlation Spectroscopy Editing of <sup>1</sup> H NMR Spectra of Biofluids: Application to Drug Metabolite Profile Identification and Enhanced Information Recovery. Analytical Chemistry, 2009, 81, 6458-6466.	3.2	38
172	Bile UPLCâ€MS fingerprinting and bile acid fluxes during human liver transplantation. Electrophoresis, 2011, 32, 2063-2070.	1.3	38
173	Evaluation of High Resolution Magic-Angle Coil Spinning NMR Spectroscopy for Metabolic Profiling of Nanoliter Tissue Biopsies. Analytical Chemistry, 2012, 84, 3843-3848.	3.2	38
174	Internal temperature calibration for1H NMR spectroscopy studies of blood plasma and other biofluids. NMR in Biomedicine, 1994, 7, 243-247.	1.6	37
175	Direct Characterization of Drug Glucuronide Isomers in Human Urine by HPLCâ~'NMR Spectroscopy:Â Application to the Positional Isomers of 6,11-Dihydro-11-oxodibenz[b,e]oxepin-2-acetic Acid Glucuronide. Analytical Chemistry, 1996, 68, 2832-2837.	3.2	37
176	NMR Spectroscopic and Theoretical Chemistry Studies on the Internal Acyl Migration Reactions of the 1-O-Acyl-β-d-glucopyranuronate Conjugates of 2-, 3-, and 4-(Trifluoromethyl)benzoic Acids. Chemical Research in Toxicology, 1996, 9, 1414-1424.	1.7	37
177	Workflow for Integrated Processing of Multicohort Untargeted <sup>1</sup> H NMR Metabolomics Data in Large-Scale Metabolic Epidemiology. Journal of Proteome Research, 2016, 15, 4188-4194.	1.8	37
178	Liquid chromatography–mass spectrometry methods for urinary biomarker detection in metabonomic studies with application to nutritional studies. Biomedical Chromatography, 2010, 24, 737-743.	0.8	36
179	Cluster Analysis Statistical Spectroscopy Using Nuclear Magnetic Resonance Generated Metabolic Data Sets from Perturbed Biological Systems. Analytical Chemistry, 2009, 81, 6581-6589.	3.2	36
180	Investigation of the human metabolism of antipyrine using coupled liquid chromatography and nuclear magnetic resonance spectroscopy of urine. Biomedical Applications, 1993, 617, 324-328.	1.7	35

#	Article	IF	CITATIONS
181	Selective Inverse-Detected Long-Range HeteronuclearJ-Resolved NMR Spectroscopy and Its Application to the Measurement of3JCH. Journal of Magnetic Resonance Series B, 1995, 109, 275-283.	1.6	35
182	Characterization of Metabolites in IntactStreptomyces citricolorCulture Supernatants Using High-Resolution Nuclear Magnetic Resonance and Directly Coupled High-Pressure Liquid Chromatography–Nuclear Magnetic Resonance Spectroscopy. Analytical Biochemistry, 1999, 270, 220-230.	1,1	34
183	Pharmacometabonomic Investigation of Dynamic Metabolic Phenotypes Associated with Variability in Response to Galactosamine Hepatotoxicity. Journal of Proteome Research, 2012, 11, 2427-2440.	1.8	34
184	Application of Directly Coupled HPLC-NMR-MS/MS to the Identification of Metabolites of 5-Trifluoromethylpyridone (2-Hydroxy-5-trifluoromethylpyridine) in Hydroponically Grown Plants. Journal of Agricultural and Food Chemistry, 2000, 48, 42-46.	2.4	33
185	Evaluation of metabolic variation in normal rat strains from a statistical analysis of 1H NMR spectra of urine. Journal of Pharmaceutical and Biomedical Analysis, 2004, 36, 823-833.	1.4	33
186	Pharmacometabonomic Characterization of Xenobiotic and Endogenous Metabolic Phenotypes That Account for Inter-individual Variation in Isoniazid-Induced Toxicological Response. Journal of Proteome Research, 2012, 11, 4630-4642.	1.8	33
187	Chiral Metabonomics: 1H NMR-Based Enantiospecific Differentiation of Metabolites in Human Urine via Direct Cosolvation with β-Cyclodextrin. Analytical Chemistry, 2012, 84, 2868-2874.	3.2	33
188	Impurity profiling in bulk pharmaceutical batches using 19F NMR spectroscopy and distinction between monomeric and dimeric impurities by NMR-based diffusion measurements. Journal of Pharmaceutical and Biomedical Analysis, 1999, 19, 511-517.	1.4	32
189	Directly Coupled Chiral HPLCâ^'NMR and HPLCâ^'CD Spectroscopy as Complementary Methods for Structural and Enantiomeric Isomer Identification:Â Application to Atracurium Besylate. Analytical Chemistry, 1999, 71, 2838-2843.	3.2	32
190	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.	3.2	32
191	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.	3.2	32
192	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.	3.2	32
193	A comparison of human serum and plasma metabolites using untargeted 1H NMR spectroscopy and UPLC-MS. Metabolomics, 2018, 14, 32.	1.4	31
194	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. Archives of Toxicology, 1994, 69, 99-110.	1.9	29
195	NMR spectroscopic studies on the haemolymph of the tobacco hornworm, Manduca sexta: assignment of 1H and 13C NMR spectra. Insect Biochemistry and Molecular Biology, 1999, 29, 795-805.	1.2	29
196	Application of Directly Coupled HPLC NMR to Separation and Characterization of Lipoproteins from Human Serum. Analytical Chemistry, 2001, 73, 1084-1090.	3.2	29
197	1H NMR-based metabonomics for investigating diabetes. Future Medicinal Chemistry, 2009, 1, 737-747.	1.1	29
198	Optimized Phenotypic Biomarker Discovery and Confounder Elimination via Covariate-Adjusted Projection to Latent Structures from Metabolic Spectroscopy Data. Journal of Proteome Research, 2018, 17, 1586-1595.	1.8	29

#	Article	IF	CITATIONS
199	Investigation of the Metabolite Variation in Control Rat Urine Using 1H NMR Spectroscopy. Analytical Biochemistry, 2001, 291, 17-26.	1.1	28
200	Quantitation in gradient high performance liquid chromatography/inductively coupled mass spectrometry investigated using diclofenac and chlorpromazine. Rapid Communications in Mass Spectrometry, 2002, 16, 245-247.	0.7	28
201	Structure and conformation of 4,4′-bipyridyl by nuclear magnetic resonance spectroscopy of a nematic solution. Journal of the Chemical Society Perkin Transactions II, 1975, , 1541-1544.	0.9	27
202	Recent advances in high-resolution NMR spectroscopic methods in bioanalytical chemistry. TrAC - Trends in Analytical Chemistry, 1997, 16, 190-200.	5.8	26
203	Statistical Total Correlation Spectroscopy Scaling for Enhancement of Metabolic Information Recovery in Biological NMR Spectra. Analytical Chemistry, 2012, 84, 1083-1091.	3.2	26
204	Improving Visualization and Interpretation of Metabolome-Wide Association Studies: An Application in a Population-Based Cohort Using Untargeted <sup>1</sup> H NMR Metabolic Profiling. Journal of Proteome Research, 2017, 16, 3623-3633.	1.8	26
205	High-performance liquid chromatography directly coupled to 19F and 1H NMR for the analysis of mixtures of isomeric ester glucuronide conjugates of trifluoromethylbenzoic acids. Journal of Chromatography A, 1996, 728, 377-385.	1.8	25
206	NMR and HPLC-NMR spectroscopic studies of futile deacetylation in paracetamol metabolites in rat and man. Journal of Pharmaceutical and Biomedical Analysis, 1997, 15, 901-910.	1.4	25
207	The potential of 19F NMR spectroscopy for rapid screening of cell cultures for models of mammalian drug metabolism. Analyst, The, 2001, 126, 2103-2106.	1.7	25
208	LC-1H NMR used for determination of the elution order of S-naproxen glucuronide isomers in two isocratic reversed-phase LC-systems. Journal of Pharmaceutical and Biomedical Analysis, 2001, 24, 477-485.	1.4	25
209	Synthesis, transacylation kinetics and computational chemistry of a set of arylacetic acid 1β-O-acyl glucuronides. Organic and Biomolecular Chemistry, 2009, 7, 2525.	1.5	25
210	A Metabolic Entropy Approach for Measurements of Systemic Metabolic Disruptions in Patho-Physiological States. Journal of Proteome Research, 2010, 9, 3537-3544.	1.8	25
211	Untargeted Metabolome Quantitative Trait Locus Mapping Associates Variation in Urine Glycerate to Mutant Glycerate Kinase. Journal of Proteome Research, 2012, 11, 631-642.	1.8	25
212	Processing and Modeling of Nuclear Magnetic Resonance (NMR) Metabolic Profiles. Methods in Molecular Biology, 2011, 708, 365-388.	0.4	25
213	Application of Directly Coupled High-performance Liquid Chromatography–Nuclear Magnetic Resonance–Mass Spectrometry to the Detection and Characterisation of the Metabolites of 2-Bromo-4-trifluoromethylaniline in Rat Urine. Analytical Communications, 1997, 34, 37-39.	2.2	24
214	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. Chromatographia, 2002, 55, S9-S13.	0.7	24
215	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. Analytical Chemistry, 2008, 80, 4876-4885.	3.2	24
216	Low Volume in Vitro Diagnostic Proton NMR Spectroscopy of Human Blood Plasma for Lipoprotein and Metabolite Analysis: Application to SARS-CoV-2 Biomarkers. Journal of Proteome Research, 2021, 20, 1415-1423.	1.8	24

#	Article	IF	CITATIONS
217	Effect of vibrational averaging on the quadrupole coupling constant of deuterium in 4-[2H1] pyridine determined from1H–{2H} INDOR n.m.r. of a partially oriented sample. Journal of the Chemical Society, Faraday Transactions 2, 1975, 71, 579-585.	1.1	23
218	Application of the one-dimensional TOCSY pulse sequence in 750 MHz 1H-NMR spectroscopy for assignment of endogenous metabolite resonances in biofluids. Journal of Pharmaceutical and Biomedical Analysis, 1994, 12, 613-618.	1.4	23
219	Metabonomics and Metabolomics Techniques and Their Applications in Mammalian Systems. , 2007, , 1-33.		23
220	Multiplatform serum metabolic phenotyping combined with pathway mapping to identify biochemical differences in smokers. Bioanalysis, 2016, 8, 2023-2043.	0.6	22
221	NMR spectroscopic studies of the transacylation reactivity of ibuprofen 1-β-O-acyl glucuronide. Journal of Pharmaceutical and Biomedical Analysis, 2006, 41, 1002-1006.	1.4	21
222	Seminal Oligouridinosis: Low Uridine Secretion as a Biomarker for Infertility in Spinal Neurotrauma. Clinical Chemistry, 2008, 54, 2063-2066.	1.5	21
223	Application of CE–MS to a metabonomics study of human urine from cigarette smokers and non-smokers. Bioanalysis, 2014, 6, 2733-2749.	0.6	21
224	A Unified Conceptual Framework for Metabolic Phenotyping in Diagnosis and Prognosis. Trends in Pharmacological Sciences, 2019, 40, 763-773.	4.0	21
225	Quantitative structure chromatography relationships in reversed-phase high performance liquid chromatography: Prediction of retention behaviour using theoretically derived molecular properties. Chromatographia, 1993, 37, 241-249.	0.7	20
226	Synthesis of a series of phenylacetic acid 1-β-O-acyl glucosides and comparison of their acyl migration and hydrolysis kinetics with the corresponding acyl glucuronides. Organic and Biomolecular Chemistry, 2011, 9, 926-934.	1.5	20
227	Selective Detection of 1H NMR Resonances of CHn Groups Using a Heteronuclear Maximum-Quantum Filter and Pulsed Field Gradients. Journal of Magnetic Resonance Series B, 1995, 106, 270-278.	1.6	19
228	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. Biomedical Applications, 1996, 685, 113-122.	1.7	19
229	Directly-coupled HPLC-NMR spectroscopic studies of metabolism and futile deacetylation of phenacetin in the rat. Journal of Pharmaceutical and Biomedical Analysis, 1999, 20, 865-873.	1.4	19
230	Hepatotoxin-induced hypertyrosinemia and its toxicological significance. Archives of Toxicology, 2007, 81, 201-210.	1.9	19
231	Topological analysis of metabolic networks integrating co-segregating transcriptomes and metabolomes in type 2 diabetic rat congenic series. Genome Medicine, 2016, 8, 101.	3.6	19
232	Title is missing!. ScienceAsia, 2008, 34, 279.	0.2	19
233	Protonation equilibria of cardiotonic polyaza heterocycles. Journal of the Chemical Society Perkin Transactions II, 1988, , 1839.	0.9	18
234	Recovery of Underwater Resonances by Magnetization Transferred NMR Spectroscopy (RECUR-NMR). Journal of Magnetic Resonance, 2001, 153, 133-137.	1.2	18

#	Article	IF	CITATIONS
235	HPLC–NMR–MS: past, present and future. Drug Discovery Today, 2003, 8, 1021-1022.	3.2	18
236	<i>J</i> -Resolved <sup>1</sup> H NMR 1D-Projections for Large-Scale Metabolic Phenotyping Studies: Application to Blood Plasma Analysis. Analytical Chemistry, 2017, 89, 11405-11412.	3.2	18
237	Can joint fluid metabolic profiling (or "metabonomicsâ€ <del>)</del> reveal biomarkers for osteoarthritis and inflammatory joint disease?. Bone and Joint Research, 2020, 9, 108-119.	1.3	18
238	Selective Detection of 1H NMR Resonances of 13CHn Groups Using Two-Dimensional Maximum-Quantum Correlation Spectroscopy. Journal of Magnetic Resonance Series A, 1995, 112, 208-219.	1.6	17
239	First example of hepatocyte transplantation to alleviate ornithine transcarbamylase deficiency, monitored by NMR-based metabonomics. Bioanalysis, 2009, 1, 1527-1535.	0.6	17
240	J-Edited DIffusional Proton Nuclear Magnetic Resonance Spectroscopic Measurement of Glycoprotein and Supramolecular Phospholipid Biomarkers of Inflammation in Human Serum. Analytical Chemistry, 2022, 94, 1333-1341.	3.2	17
241	An assessment of simple theories of chemical shifts of aromatic protons as applied to substituted naphthalenes. Journal of the Chemical Society Perkin Transactions II, 1973, , 611.	0.9	16
242	Deuterium NMR spectroscopy of biofluids for the identification of drug metabolites: Application to N,N-dimethylformamide. Journal of Pharmaceutical and Biomedical Analysis, 1993, 11, 687-692.	1.4	16
243	Determination of the relative NH proton lifetimes of the peptide analogue viomycin in aqueous solution by NMR-based diffusion measurement. Journal of Biomolecular NMR, 1999, 13, 25-30.	1.6	16
244	High-performance liquid chromatography/inductively coupled plasma mass spectrometry with iodine-specific detection for profiling the metabolites produced in the earthwormEisenia veneta by exposure to 2-fluoro-4-iodoaniline. Rapid Communications in Mass Spectrometry, 2003, 17, 1855-1858.	0.7	16
245	NMR of biofluids: Detection of 2H-acetate and 2H-formate in urine as an indicator of microbiological contamination. Journal of Pharmaceutical and Biomedical Analysis, 1993, 11, 169-172.	1.4	15
246	Two-dimensional1H1H and13C1H maximum-quantum correlation NMR spectroscopy with application to the assignment of the NMR spectra of the bile salt sodium taurocholate. Magnetic Resonance in Chemistry, 1995, 33, 212-219.	1.1	15
247	750 MHz HPLC-NMR spectroscopic identification of rat microsomal metabolites of phenoxypyridines. Journal of Pharmaceutical and Biomedical Analysis, 1997, 16, 481-489.	1.4	15
248	Enhanced effect of magnetic field gradients using multiple quantum NMR spectroscopy applied to self-diffusion coefficient measurement. Molecular Physics, 1998, 93, 913-920.	0.8	15
249	Sites of protonation in cardiotonic polyazaindolizines by NMR spectroscopy. Magnetic Resonance in Chemistry, 1991, 29, 468-475.	1.1	14
250	Hyphenated methods. Analytical Proceedings, 1993, 30, 390.	0.4	14
251	Metabonomic investigations into the global biochemical sequelae of exposure to the pancreatic toxin 1â€eyanoâ€2â€hydroxyâ€3â€butene in the rat. Magnetic Resonance in Chemistry, 2009, 47, S26-35.	1.1	14
252	Proton shielding anisotropy in benzene. Molecular Physics, 1970, 19, 285-287.	0.8	13

#	Article	IF	CITATIONS
253	Conformation and reorientation of acetophenone in solution. A proton and deuterium magnetic resonance study in a nematic solvent. Journal of the Chemical Society, Faraday Transactions 2, 1976, 72, 1365.	1.1	13
254	Probing Molecular Dynamics in Chromatographic Systems Using High-Resolution1H Magic-Angle-Spinning NMR Spectroscopy:A Interaction betweenp-Xylene and C18-Bonded Silica. Analytical Chemistry, 2004, 76, 3023-3028.	3.2	13
255	A high-performance liquid chromatography and nuclear magnetic resonance spectroscopy-based analysis of commercially available praziquantel tablets. Journal of Pharmaceutical and Biomedical Analysis, 2007, 45, 263-267.	1.4	13
256	Application of the FLIPSY Pulse Sequence for Increased Sensitivity in1H NMR-Based Metabolic Profiling Studies. Analytical Chemistry, 2008, 80, 3365-3371.	3.2	13
257	Chemical shift calibration of <sup>1</sup> H MAS NMR liver tissue spectra exemplified using a study of glycine protection of galactosamine toxicity. Magnetic Resonance in Chemistry, 2009, 47, S47-53.	1.1	13
258	Highâ€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. Rapid Communications in Mass Spectrometry, 2010, 24, 3043-3051.	0.7	13
259	Non-linear modeling of 1H NMR metabonomic data using kernel-based orthogonal projections to latent structures optimized by simulated annealing. Analytica Chimica Acta, 2011, 705, 72-80.	2.6	13
260	Exploration of Human Serum Lipoprotein Supramolecular Phospholipids Using Statistical Heterospectroscopy in <i>n</i> -Dimensions (SHY- <i>n</i> ): Identification of Potential Cardiovascular Risk Biomarkers Related to SARS-CoV-2 Infection. Analytical Chemistry, 2022, 94, 4426-4436.	3.2	13
261	Studies on the effects ofl(αS,5S)-α-amino-3-chloro-4,5-dihydro-5-isoxazoleacetic acid (AT-125) on 4-aminophenol-induced nephrotoxicity in the Fischer 344 rat. Archives of Toxicology, 1993, 67, 696-705.	1.9	12
262	NMR spectroscopic diffusion, chemical shift and linewidth measurements of low-affinity binding of ibuprofen enantiomers to human serum albumin. Magnetic Resonance in Chemistry, 1999, 37, 269-273.	1.1	12
263	Spectroscopic and statistical methods in metabonomics. Bioanalysis, 2009, 1, 1559-1578.	0.6	12
264	Measurement of inter-proton distances from cross-relaxation rates determined by a selective null inversion-recovery NMR method. Magnetic Resonance in Chemistry, 1992, 30, 173-176.	1.1	11
265	1H NMR dipolar relaxation times and the derivation of internuclear distance. Concepts in Magnetic Resonance, 1996, 8, 161-173.	1.3	11
266	Investigation of the feasibility of directly-coupled HPLC-NMR with 2H detection with application to the metabolism of N-dimethylformamide-d7. Journal of Pharmaceutical and Biomedical Analysis, 1997, 16, 1-5.	1.4	11
267	Diffusion Coefficient Measurement by High Resolution NMR Spectroscopy: Biochemical and Pharmaceutical Applications. Reviews in Analytical Chemistry, 1999, 18, .	1.5	11
268	Peer Reviewed: Advancing Hyphenated Chromatographic Systems Analytical Chemistry, 2000, 72, 534 A-542 A.	3.2	11
269	Conformations of 3,5-dichloroanisole and 3,5-dibromoacetophenone determined from 1H nuclear magnetic resonance spectra of nematic solutions. Journal of the Chemical Society Perkin Transactions II, 1976, , 805.	0.9	10
270	High resolution proton nuclear magnetic resonance studies of interaction between deoxyhaemoglobin and small molecules. Dithionite and diphosphoglycerate. Journal of the Chemical Society Faraday Transactions I, 1979, 75, 2851.	1.0	10

#	Article	IF	CITATIONS
271	An adventitious synthesis of a 5-methylimidazo[4,5-c]pyridine derivative. Tetrahedron Letters, 1986, 27, 5997-6000.	0.7	10
272	Observation of Separate J-Resolved 1H-NMR Spectra from CH, CH2, and CH3 Groups Using a Maximum-Quantum Filter. Journal of Magnetic Resonance Series A, 1995, 113, 251-256.	1.6	10
273	Determination of the tautomeric equilibria of pyridoyl benzoyl β-diketones in the liquid and solid state through the use of deuterium isotope effects on 1H and 13C NMR chemical shifts and spin coupling constants. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 107-112.	2.0	10
274	Structure of pentafluorobenzaldehyde determined from nuclear magnetic resonance spectra of nematic solutions. Journal of the Chemical Society Perkin Transactions II, 1975, , 1508.	0.9	9
275	Three-Dimensional Maximum-Quantum Correlation HMQC NMR Spectroscopy (3D MAXY-HMQC). Journal of Magnetic Resonance, 1997, 129, 67-73.	1.2	9
276	Urinary metabolites of 2-bromoethanamine identified by stable isotope labelling: evidence for carbamoylation and glutathione conjugation. Xenobiotica, 2011, 41, 144-154.	0.5	9
277	Improved Spatial Resolution of Metabolites in Tissue Biopsies Using High-Resolution Magic-Angle-Spinning Slice Localization NMR Spectroscopy. Analytical Chemistry, 2020, 92, 11516-11519.	3.2	9
278	Orientation studies by N.M.R. spectroscopy using a lyotropic liquid crystal solvent. Molecular Physics, 1971, 20, 937-940.	0.8	8
279	Assignment of the 1H, 19F, and 13C NMR spectra of 2-deoxy-2-fluoro-d-ribose and characterisation of the isomeric equilibrium. Carbohydrate Research, 1996, 284, 51-60.	1.1	8
280	Continuous bond rotation models for the conformational analysis of the methoxy groups in 1,2-dimethoxy- and 1,2,3-trimethoxy-benzene using dipolar couplings obtained from the NMR spectra of oriented samples in nematic liquid crystalline solutions. Journal of the Chemical Society Perkin Transactions II, 1998, , 1211-1218.	0.9	8
281	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.	1.0	8
282	Structure of 2,3,5,6-tetrafluoroanisole determined from the analysis of a nuclear magnetic resonance spectrum of a nematic solution. Journal of the Chemical Society Perkin Transactions II, 1975, , 1794.	0.9	7
283	Proton, carbon-13 and proton-(deuterium) INDOR n.m.r. spectra of isotopically labelled acetaldehyde dissolved in a nematic phase. Journal of the Chemical Society, Faraday Transactions 2, 1975, 71, 586.	1.1	7
284	Structural investigation of the Îallyl group in (Îallyl)tetracarbonylrhenium by nematic-phase nuclear magnetic resonance spectroscopy. Journal of the Chemical Society Dalton Transactions, 1975, , 1264.	1.1	7
285	Structures of 1,3,5-trichloro- and 1,3,5-trichlorotrifluorobenzene derived from n.m.r. spectra of nematic solutions. Journal of the Chemical Society, Faraday Transactions 2, 1976, 72, 1436.	1.1	7
286	Automatic Recognition of Multiplet Patterns and Measurement of Coupling Constants in NMR and EPR Spectra through the Application of Maximum-Entropy Deconvolution. Journal of Magnetic Resonance Series A, 1996, 119, 191-196.	1.6	7
287	2.7.5. HPLC/NMR and related hyphenated NMR methods. Progress in Pharmaceutical and Biomedical Analysis, 2000, 4, 299-322.	0.1	7
288	An investigation of solid-state phase transitions in 1- and 2-adamantanol by 13C CP-MAS NMR. Thermochimica Acta, 1991, 179, 295-300.	1.2	6

#	Article	IF	CITATIONS
289	Quantitative Investigation of Probabilistic Spectral Processing Methods Using Simulated NMR Data. Applied Spectroscopy, 2001, 55, 1214-1224.	1.2	6
290	Highâ€resolution <sup>1</sup> H NMR spectroscopic investigation of a chick embryo model of neural tube development. Magnetic Resonance in Chemistry, 2009, 47, S62-7.	1.1	6
291	Development of quantitative structure-metabolism (QSMR) relationships for substituted anilines based on computational chemistry. Xenobiotica, 2013, 43, 792-802.	0.5	6
292	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
293	Investigation of water environments in a C18 bonded silica phase using 1H magic angle spinning (MAS) nuclear magnetic resonance (NMR) spectroscopy. Analyst, The, 2001, 126, 548-550.	1.7	5
294	Biomedical and Pharmaceutical Applications of HPLC–NMR and HPLC–NMR–MS. , 0, , 45-87.		5
295	NMR and MS urinary metabolic phenotyping in kidney diseases is fit-for-purpose in the presence of a protease inhibitor. Molecular Omics, 2019, 15, 39-49.	1.4	5
296	Kinetic modelling of acyl glucuronide and glucoside reactivity and development of structure–property relationships. Organic and Biomolecular Chemistry, 2020, 18, 1389-1401.	1.5	5
297	Differences between infected and noninfected synovial fluid. Bone and Joint Research, 2021, 10, 85-95.	1.3	5
298	Biofluids Studied By NMR. , 1999, , 98-116.		4
299	NMR Spectrometers. , 2010, , 1872-1880.		4
300	The influence of sample collection, handling and low temperature storage upon NMR metabolic profiling analysis in human synovial fluid. Journal of Pharmaceutical and Biomedical Analysis, 2021, 197, 113942.	1.4	4
301	Studies of the biochemical toxicology of uranyl nitratein the rat. Archives of Toxicology, 1994, 68, 43.	1.9	4
302	Recent Advances in Editing and Selective Detection Methods for 1 H NMR Spectroscopy. Current Organic Chemistry, 2001, 5, 351-371.	0.9	4
303	Structure and conformation of 4-nitrophenyl acetate from proton nuclear magnetic resonance of nematic solutions. Journal of the Chemical Society Perkin Transactions II, 1977, , 1383.	0.9	3
304	The 1H nuclear magnetic resonance spectra of 6-substituted bicyclo[3.1.0] hex-2-enes. Journal of the Chemical Society Perkin Transactions II, 1982, , 651.	0.9	3
305	Solid state 13C NMR and phase transitions in hydroxyadamantanes. Thermochimica Acta, 1989, 146, 361-364.	1.2	3

Overview of NMR-Based Metabonomics. , 2010, , 2058-2068.

3

#	Article	IF	CITATIONS
307	The Development of Metabolic Phenotyping—A Historical Perspective. , 2016, , 17-48.		3
308	Conclusions from NMR on the preferred direction of attack during quaternisation of 1-benzyl-tetrahydroisoquinolines. Tetrahedron, 1980, 36, 2157-2159.	1.0	2
309	Intramolecular acetalisation of naphthoquinones. Journal of the Chemical Society Perkin Transactions 1, 1982, , 1933.	0.9	2
310	Studies of tautomerism and protonation in 2-aryl-1H-imidazo[1,2-a]imidazole derivatives using1H and13C NMR. Magnetic Resonance in Chemistry, 1991, 29, 1147-1151.	1.1	2
311	Biomedical applications of directly-coupled chromatography–nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry (MS). Handbook of Analytical Separations, 2003, , 293-329.	0.8	2
312	Biofluids Studied by NMR Spectroscopy*. , 2010, , 128-141.		2
313	Response to Comment on "Optimized Preprocessing of Ultra-Performance Liquid Chromatography/Mass Spectrometry Urinary Metabolic Profiles for Improved Information Recoveryâ€: Analytical Chemistry, 2011, 83, 9721-9722.	3.2	2
314	An Overview of Metabolic Phenotyping and Its Role in Systems Biology. , 2019, , 1-51.		2
315	Metabonomics: Metabolic processes studied by NMR spectroscopy of biofluids. , 0, .		2
316	Observation of solid-state phase changes in adamantanols using 13C CP-MAS NMR. Thermochimica Acta, 1994, 232, 171-176.	1.2	1
317	Characterisation of the conformational and tautomeric properties of benzylamino derivatives of 1,4-diphenyl-2-butene-1,4-dione using NMR spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 1521-1525.	2.0	1
318	NMR-based Metabonomics Techniques and Applications. , 2008, , 1377-1385.		1
319	A Survey of Metabonomics Approaches for Disease Characterisation. , 2007, , 413-442.		1
320	The Metabolic Window into Systems Biology. Journal of Proteome Research, 2007, 6, 433-433.	1.8	1
321	An Overview of Metabonomics Techniques and Applications. , 0, , 1503-1524.		1
322	Pharmacometabonomics and Predictive Metabonomics. , 2016, , 137-165.		1
323	The -Omics in Drug Development. , 2011, , 145-173.		1
324	Global Systems Biology Through Integration of "Omics―Results. , 2007, , 533-555.		1

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#	Article	IF	CITATIONS
325	NMR-based Metabolic Phenotyping Techniques and Applications. , 2017, , 1-25.		1
326	NMR — from chemistry to medicine. Nature, 1983, 303, 265-265.	13.7	0
327	Measurement of longitudinal relaxation times in crowded1H NMR spectra using one- and two-dimensional maximum quantum (MAXY) NMR spectroscopy. Molecular Physics, 2001, 99, 1701-1707.	0.8	Ο
328	The Development of a Metabonomic-Based Drug Safety Testing Paradigm. , 0, , 309-343.		0
329	NMR-Based Metabolic Phenotyping: An Overview â~†. , 2018, , 375-375.		Ο
330	Conception, Implementation and Operation of Large-Scale Metabolic Phenotyping Centres: Phenome Centres. , 2019, , 385-405.		0
331	Metabolic Phenotyping: History, Status, and Prospects. , 2019, , 571-583.		0
332	Metabonomics and Its Role in Disease Diagnosis. , 2004, , 797-802.		0
333	An Overview of Metabonomics. , 2005, , 1-26.		Ο
334	Future Visions for Clinical Metabolic Phenotyping. , 2016, , 369-388.		0
335	NMR-Based Metabolic Phenotyping Techniques and Applications. , 2018, , 2163-2187.		0
336	Application of novel solid phase extraction-NMR protocols for metabolic profiling of human urine. Faraday Discussions, 2019, 218, 395-416.	1.6	0