David Scott Wishart

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3931240/publications.pdf

Version: 2024-02-01

419 papers	86,667 citations	1296 112 h-index	448 280 g-index
429 all docs	429 docs citations	429 times ranked	103035 citing authors

#	Article	IF	Citations
1	NP-MRD: the Natural Products Magnetic Resonance Database. Nucleic Acids Research, 2022, 50, D665-D677.	6.5	39
2	HMDB 5.0: the Human Metabolome Database for 2022. Nucleic Acids Research, 2022, 50, D622-D631.	6.5	736
3	Metabolomics in Exercise and Sports: A Systematic Review. Sports Medicine, 2022, 52, 547-583.	3.1	34
4	Emerging technologies and their impact on regulatory science. Experimental Biology and Medicine, 2022, 247, 1-75.	1.1	22
5	Urinary metabolomics to develop predictors for pediatric acute kidney injury. Pediatric Nephrology, 2022, 37, 2079-2090.	0.9	4
6	Metabolomic Fingerprint of Behavioral Changes in Response to Full-Spectrum Cannabis Extracts. Frontiers in Pharmacology, 2022, 13, 831052.	1.6	2
7	Blood Metabolomic Phenotyping of Dry Cows Could Predict the High Milk Somatic Cells in Early Lactationâ€"Preliminary Results. Dairy, 2022, 3, 59-77.	0.7	3
8	Identification of Serum-Predictive Biomarkers for Subclinical Mastitis in Dairy Cows and New Insights into the Pathobiology of the Disease. Journal of Agricultural and Food Chemistry, 2022, 70, 1724-1746.	2.4	5
9	Combination of mouse prion protein with detoxified lipopolysaccharide triggers colon genes related to inflammatory, antibacterial, and apoptotic responses. Research in Veterinary Science, 2022, 144, 98-107.	0.9	1
10	Metabolomics and the Multi-Omics View of Cancer. Metabolites, 2022, 12, 154.	1.3	17
11	Systemic inflammation and metabolic disturbances underlie inpatient mortality among ill children with severe malnutrition. Science Advances, 2022, 8, eabj6779.	4.7	14
12	BioTransformer 3.0â€"a web server for accurately predicting metabolic transformation products. Nucleic Acids Research, 2022, 50, W115-W123.	6.5	33
13	The impact of methodological choices when developing predictive models using urinary metabolite data. Statistics in Medicine, 2022, , .	0.8	0
14	Advances in Metabolomics-Driven Diagnostic Breeding and Crop Improvement. Metabolites, 2022, 12, 511.	1.3	9
15	Predictive blood biomarkers of sheep pregnancy and litter size. Scientific Reports, 2022, 12, .	1.6	4
16	Acylcarnitines: Nomenclature, Biomarkers, Therapeutic Potential, Drug Targets, and Clinical Trials. Pharmacological Reviews, 2022, 74, 506-551.	7.1	106
17	MarkerDB: an online database of molecular biomarkers. Nucleic Acids Research, 2021, 49, D1259-D1267.	6.5	64
18	Predicting PAMPA permeability using the 3D-RISM-KH theory: are we there yet?. Journal of Computer-Aided Molecular Design, 2021, 35, 261-269.	1.3	6

#	Article	IF	Citations
19	Food Constituent and Food Metabolite Databases. , 2021, , 2-18.		2
20	Cloning and high-level expression of monomeric human superoxide dismutase 1 (SOD1) and its interaction with pyrimidine analogs. PLoS ONE, 2021, 16, e0247684.	1.1	1
21	CpG-ODN induced antimicrobial immunity in neonatal chicks involves a substantial shift in serum metabolic profiles. Scientific Reports, 2021, 11, 9028.	1.6	3
22	A Comprehensive Targeted Metabolomics Assay for Crop Plant Sample Analysis. Metabolites, 2021, 11, 303.	1.3	15
23	CyProduct: A Software Tool for Accurately Predicting the Byproducts of Human Cytochrome P450 Metabolism. Journal of Chemical Information and Modeling, 2021, 61, 3128-3140.	2.5	14
24	Chemical language models enable navigation in sparsely populated chemical space. Nature Machine Intelligence, 2021, 3, 759-770.	8.3	48
25	Targeted metabolomics identifies high performing diagnostic and prognostic biomarkers for COVID-19. Scientific Reports, 2021, 11, 14732.	1.6	41
26	A Cross-Platform Metabolomics Comparison Identifies Serum Metabolite Signatures of Liver Fibrosis Progression in Chronic Hepatitis C Patients. Frontiers in Molecular Biosciences, 2021, 8, 676349.	1.6	11
27	Immunometabolic signatures predict risk of progression to sepsis in COVID-19. PLoS ONE, 2021, 16, e0256784.	1.1	22
28	CFM-ID 4.0: More Accurate ESI-MS/MS Spectral Prediction and Compound Identification. Analytical Chemistry, 2021, 93, 11692-11700.	3.2	151
29	Mice Treated Subcutaneously with Mouse LPS-Converted PrPres or LPS Alone Showed Brain Gene Expression Profiles Characteristic of Prion Disease. Veterinary Sciences, 2021, 8, 200.	0.6	1
30	A Targeted Serum Metabolomics GC-MS Approach Identifies Predictive Blood Biomarkers for Retained Placenta in Holstein Dairy Cows. Metabolites, 2021, 11, 633.	1.3	5
31	A longitudinal dataset of incidence and intervention policy impacts regarding the COVID-19 pandemic in Canadian provinces. Data in Brief, 2021, 38, 107381.	0.5	2
32	A Multi-Platform Metabolomics Approach Identifies Urinary Metabolite Signatures That Differentiate Ketotic From Healthy Dairy Cows. Frontiers in Veterinary Science, 2021, 8, 595983.	0.9	12
33	Exploring Biological Impacts of Prenatal Nutrition and Selection for Residual Feed Intake on Beef Cattle Using Omics Technologies: A Review. Frontiers in Genetics, 2021, 12, 720268.	1.1	2
34	A deep generative model enables automated structure elucidation of novel psychoactive substances. Nature Machine Intelligence, 2021, 3, 973-984.	8.3	28
35	A Canadian Study of Cisplatin Metabolomics and Nephrotoxicity (ACCENT): A Clinical Research Protocol. Canadian Journal of Kidney Health and Disease, 2021, 8, 205435812110577.	0.6	1
36	Perspective: Dietary Biomarkers of Intake and Exposureâ€"Exploration with Omics Approaches. Advances in Nutrition, 2020, 11, 200-215.	2.9	79

#	Article	IF	Citations
37	PathBank: a comprehensive pathway database for model organisms. Nucleic Acids Research, 2020, 48, D470-D478.	6.5	83
38	Serum metabolic fingerprinting of pre-lameness dairy cows by GCâ€“MS reveals typical profiles that can identify susceptible cows. Journal of Proteomics, 2020, 213, 103620.	1.2	8
39	Mass-spec-based urinary metabotyping around parturition identifies screening biomarkers for subclinical mastitis in dairy cows. Research in Veterinary Science, 2020, 129, 39-52.	0.9	12
40	Gut Microenvironment and Bacterial Invasion in Paediatric Inflammatory Bowel Diseases. Journal of Pediatric Gastroenterology and Nutrition, 2020, 71, 624-632.	0.9	12
41	Workshop report: Toward the development of a human whole stool reference material for metabolomic and metagenomic gut microbiome measurements. Metabolomics, 2020, 16, 119.	1.4	12
42	Serum Metabolite Biomarkers for Predicting Residual Feed Intake (RFI) of Young Angus Bulls. Metabolites, 2020, 10, 491.	1.3	18
43	Excretory/Secretory Metabolome of the Zoonotic Roundworm Parasite Toxocara canis. Biomolecules, 2020, 10, 1157.	1.8	12
44	Metabolomics Profiling of Critically Ill Coronavirus Disease 2019 Patients: Identification of Diagnostic and Prognostic Biomarkers. , 2020, 2, e0272.		92
45	Candidate serum metabolite biomarkers of residual feed intake and carcass merit in sheep. Journal of Animal Science, 2020, 98, .	0.2	19
46	Urinary Metabolomics around Parturition Identifies Metabolite Alterations in Dairy Cows Affected Postpartum by Lameness: Preliminary Study. Dairy, 2020, 1, 2.	0.7	9
47	The Bovine Metabolome. Metabolites, 2020, 10, 233.	1.3	77
48	Serum metabolomics identifies metabolite panels that differentiate lame dairy cows from healthy ones. Metabolomics, 2020, 16, 73.	1.4	6
49	Effect of Diet on the Vitamin B Profile of Bovine Milk-Based Protein Ingredients. Foods, 2020, 9, 578.	1.9	8
50	Insights into origins and function of the unexplored majority of the reductive dehalogenase gene family as a result of genome assembly and ortholog group classification. Environmental Sciences: Processes and Impacts, 2020, 22, 663-678.	1.7	31
51	Milk Metabotyping Identifies Metabolite Alterations in the Whole Raw Milk of Dairy Cows with Lameness. Journal of Agricultural and Food Chemistry, 2020, 68, 4507-4514.	2.4	10
52	A High-Performing Plasma Metabolite Panel for Early-Stage Lung Cancer Detection. Cancers, 2020, 12, 622.	1.7	37
53	Comprehensive Targeted Metabolomic Assay for Urine Analysis. Analytical Chemistry, 2020, 92, 10627-10634.	3.2	39
54	FOBI: an ontology to represent food intake data and associate it with metabolomic data. Database: the Journal of Biological Databases and Curation, 2020, 2020, .	1.4	29

#	Article	IF	Citations
55	Value-based healthcare delivery through metabolomics-based personalized health platform. Healthcare Management Forum, 2020, 33, 126-134.	0.6	5
56	The Urinary Metabolome of Healthy Newborns. Metabolites, 2020, 10, 165.	1.3	20
57	Targeted metabolomics highlights perturbed metabolism in the brain of autism spectrum disorder sufferers. Metabolomics, 2020, 16, 59.	1.4	15
58	Metabolomic Data Exploration and Analysis with the Human Metabolome Database. Methods in Molecular Biology, 2020, 2104, 165-184.	0.4	6
59	Metabolomics for Investigating Physiological and Pathophysiological Processes. Physiological Reviews, 2019, 99, 1819-1875.	13.1	516
60	Urinary Organic Acids Increase After Clinical Stabilization of Hospitalized Children With Severe Acute Malnutrition. Food and Nutrition Bulletin, 2019, 40, 532-543.	0.5	0
61	NMR metabolomics: A look ahead. Journal of Magnetic Resonance, 2019, 306, 155-161.	1.2	129
62	NMR Spectroscopy for Metabolomics Research. Metabolites, 2019, 9, 123.	1.3	627
63	Metabolomic profiling of the excretoryâ€“secretory products of hookworm and whipworm. Metabolomics, 2019, 15, 101.	1.4	26
64	Using MetaboAnalyst 4.0 for Comprehensive and Integrative Metabolomics Data Analysis. Current Protocols in Bioinformatics, 2019, 68, e86.	25.8	1,644
65	International Ring Trial of a High Resolution Targeted Metabolomics and Lipidomics Platform for Serum and Plasma Analysis. Analytical Chemistry, 2019, 91, 14407-14416.	3.2	66
66	The role of hydration effects in 5-fluorouridine binding to SOD1: insight from a new 3D-RISM-KH based protocol for including structural water in docking simulations. Journal of Computer-Aided Molecular Design, 2019, 33, 913-926.	1.3	4
67	Preparation and characterization of a highly soluble AÎ²1-42 peptide variant. Protein Expression and Purification, 2019, 164, 105480.	0.6	5
68	Comparison of the metabolomic profiles of irritable bowel syndrome patients with ulcerative colitis patients and healthy controls: new insights into pathophysiology and potential biomarkers. Alimentary Pharmacology and Therapeutics, 2019, 49, 723-732.	1.9	37
69	Transformation of polyphenols found in pigmented gluten-free flours during in vitro large intestinal fermentation. Food Chemistry, 2019, 298, 125068.	4.2	32
70	Protocols for NMR Analysis in Livestock Metabolomics. Methods in Molecular Biology, 2019, 1996, 311-324.	0.4	8
71	A fast, sensitive, single-step colorimetric dipstick assay for quantifying ascorbic acid in urine. Analytical Biochemistry, 2019, 580, 1-13.	1.1	10
72	CFM-ID 3.0: Significantly Improved ESI-MS/MS Prediction and Compound Identification. Metabolites, 2019, 9, 72.	1.3	196

#	Article	IF	Citations
73	Systems Biology and Multi-Omics Integration: Viewpoints from the Metabolomics Research Community. Metabolites, 2019, 9, 76.	1.3	387
74	Chemical Composition of Commercial Cowâ€™s Milk. Journal of Agricultural and Food Chemistry, 2019, 67, 4897-4914.	2.4	139
75	Porous Nanophotonic Optomechanical Beams for Enhanced Mass Adsorption. ACS Sensors, 2019, 4, 1197-1202.	4.0	5
76	Editorial: metabolomic biomarkers for colorectal adenocarcinoma and in the differentiation between irritable bowel syndrome and ulcerative colitis in clinical remission â€“ confounded by the gut microbiome? Authorsâ€™ reply. Alimentary Pharmacology and Therapeutics, 2019, 49, 1088-1089.	1.9	0
77	Nonâ€invasive differentiation of nonâ€rejection kidney injury from acute rejection in pediatric renal transplant recipients. Pediatric Transplantation, 2019, 23, e13364.	0.5	6
78	Solvent Composition Effects on the Structural Properties of the AÎ²42 Monomer from the 3D-RISM-KH Molecular Theory of Solvation. Journal of Physical Chemistry B, 2019, 123, 2491-2506.	1.2	6
79	Exposome-Explorer 2.0: an update incorporating candidate dietary biomarkers and dietary associations with cancer risk. Nucleic Acids Research, 2019, 48, D908-D912.	6.5	31
80	Impact of Bovine Diet on Metabolomic Profile of Skim Milk and Whey Protein Ingredients. Metabolites, 2019, 9, 305.	1.3	20
81	Assessing the performance of genome-wide association studies for predicting disease risk. PLoS ONE, 2019, 14, e0220215.	1.1	43
82	Nutrimetabolomics: An Integrative Action for Metabolomic Analyses in Human Nutritional Studies. Molecular Nutrition and Food Research, 2019, 63, e1800384.	1.5	173
83	Edible nuts deliver polyphenols and their transformation products to the large intestine: An in vitro fermentation model combining targeted/untargeted metabolomics. Food Research International, 2019, 116, 786-794.	2.9	43
84	CEU Mass Mediator 3.0: A Metabolite Annotation Tool. Journal of Proteome Research, 2019, 18, 797-802.	1.8	104
85	BioTransformer: a comprehensive computational tool for small molecule metabolism prediction and metabolite identification. Journal of Cheminformatics, 2019, 11, 2.	2.8	269
86	PHAST, PHASTER and PHASTEST: Tools for finding prophage in bacterial genomes. Briefings in Bioinformatics, 2019, 20, 1560-1567.	3.2	151
87	First-trimester metabolomic prediction of stillbirth. Journal of Maternal-Fetal and Neonatal Medicine, 2019, 32, 3435-3441.	0.7	5
88	Automated Tools for the Analysis of 1D-NMR and 2D-NMR Spectra. Methods in Molecular Biology, 2019, 2037, 429-449.	0.4	9
89	Assessing the performance of genome-wide association studies for predicting disease risk. , 2019, 14, e0220215.		0
90	Assessing the performance of genome-wide association studies for predicting disease risk. , 2019, 14, e0220215.		0

#	Article	IF	Citations
91	Assessing the performance of genome-wide association studies for predicting disease risk. , 2019, 14, e0220215.		0
92	Assessing the performance of genome-wide association studies for predicting disease risk. , 2019, 14, e0220215.		0
93	Recommended strategies for spectral processing and post-processing of 1D 1H-NMR data of biofluids with a particular focus on urine. Metabolomics, 2018, 14, 31.	1.4	107
94	Guidelines for Biomarker of Food Intake Reviews (BFIRev): how to conduct an extensive literature search for biomarker of food intake discovery. Genes and Nutrition, 2018, 13, 3.	1.2	71
95	The role of the Human Metabolome Database in inborn errors of metabolism. Journal of Inherited Metabolic Disease, 2018, 41, 329-336.	1.7	15
96	DrugBank 5.0: a major update to the DrugBank database for 2018. Nucleic Acids Research, 2018, 46, D1074-D1082.	6.5	5,428
97	A sensitive, high-throughput LC-MS/MS method for measuring catecholamines in low volume serum. Analytica Chimica Acta, 2018, 1037, 159-167.	2.6	49
98	PAMDB: a comprehensive Pseudomonas aeruginosa metabolome database. Nucleic Acids Research, 2018, 46, D575-D580.	6.5	45
99	Evolution of renal function and urinary biomarker indicators of inflammation on serial kidney biopsies in pediatric kidney transplant recipients with and without rejection. Pediatric Transplantation, 2018, 22, e13202.	0.5	15
100	HMDB 4.0: the human metabolome database for 2018. Nucleic Acids Research, 2018, 46, D608-D617.	6.5	2,805
101	Unraveling the unknown areas of the human metabolome: the role of infrared ion spectroscopy. Journal of Inherited Metabolic Disease, 2018, 41, 367-377.	1.7	44
102	Identification of serum metabolites associated with the risk of metritis in transition dairy cows. Canadian Journal of Animal Science, 2018, 98, 525-537.	0.7	10
103	nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. Analytical Chemistry, 2018, 90, 649-656.	3.2	50
104	Rapid and reliable protein structure determination via chemical shift threading. Journal of Biomolecular NMR, 2018, 70, 33-51.	1.6	4
105	Metabolomic prediction of endometrial cancer. Metabolomics, 2018, 14, 6.	1.4	24
106	Functionalized gold nanoparticle-enhanced competitive assay for sensitive small-molecule metabolite detection using surface plasmon resonance. Analyst, The, 2018, 143, 289-296.	1.7	36
107	A Simple and Convenient Synthesis of Unlabeled and 13C-Labeled 3-(3-Hydroxyphenyl)-3-Hydroxypropionic Acid and Its Quantification in Human Urine Samples. Metabolites, 2018, 8, 80.	1.3	8
108	Non-invasive Point-of-Care Device To Diagnose Acute Mesenteric Ischemia. ACS Sensors, 2018, 3, 2296-2302.	4.0	12

#	Article	IF	Citations
109	A simple in vitro assay for assessing the efficacy, mechanisms and kinetics of anti-prion fibril compounds. Prion, 2018, 12, 280-300.	0.9	15
110	MetaboAnalyst 4.0: towards more transparent and integrative metabolomics analysis. Nucleic Acids Research, 2018, 46, W486-W494.	6.5	3,199
111	Residue-specific mobility changes in soluble oligomers of the prion protein define regions involved in aggregation. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2018, 1866, 982-988.	1.1	2
112	Growth of Malignant Non-CNS Tumors Alters Brain Metabolome. Frontiers in Genetics, 2018, 9, 41.	1.1	2
113	Pasture Feeding Changes the Bovine Rumen and Milk Metabolome. Metabolites, 2018, 8, 27.	1.3	70
114	A review on human fecal metabolomics: Methods, applications and the human fecal metabolome database. Analytica Chimica Acta, 2018, 1030, 1-24.	2.6	187
115	CypReact: A Software Tool for in Silico Reactant Prediction for Human Cytochrome P450 Enzymes. Journal of Chemical Information and Modeling, 2018, 58, 1282-1291.	2.5	54
116	Nonâ€invasive staging of chronic kidney allograft damage using urine metabolomic profiling. Pediatric Transplantation, 2018, 22, e13226.	0.5	13
117	Informatics and Data Analytics to Support Exposome-Based Discovery for Public Health. Annual Review of Public Health, 2017, 38, 279-294.	7.6	97
118	Metabotyping reveals distinct metabolic alterations in ketotic cows and identifies early predictive serum biomarkers for the risk of disease. Metabolomics, 2017, 13, 1.	1.4	35
119	Improved Glucose Homeostasis in Obese Mice Treated With Resveratrol Is Associated With Alterations in the Gut Microbiome. Diabetes, 2017, 66, 418-425.	0.3	189
120	Urinary Metabolomics for Noninvasive Detection of Antibody-Mediated Rejection in Children After Kidney Transplantation. Transplantation, 2017, 101, 2553-2561.	0.5	26
121	Targeted Metabolic Profiling of Post-Mortem Brain from Infants Who Died from Sudden Infant Death Syndrome. Journal of Proteome Research, 2017, 16, 2587-2596.	1.8	15
122	Microbiome and metabolome modifying effects of several cardiovascular disease interventions in apo-Eâ^'/â^' mice. Microbiome, 2017, 5, 30.	4.9	83
123	Peptide-based fluorescence biosensors for detection/measurement of nanoparticles. Analytical and Bioanalytical Chemistry, 2017, 409, 903-915.	1.9	4
124	Exposome-Explorer: a manually-curated database on biomarkers of exposure to dietary and environmental factors. Nucleic Acids Research, 2017, 45, D979-D984.	6.5	109
125	The compound (3-{5-[(2,5-dimethoxyphenyl)amino]-1,3,4-thiadiazolidin-2-yl}-5,8-methoxy-2H-chromen-2-one) inhibits the prion protein conversion from PrPC to PrPSc with lower IC50 in ScN2a cells. Bioorganic and Medicinal Chemistry, 2017, 25, 5875-5888.	1.4	2
126	Recombinant Incretin-Secreting Microbe Improves Metabolic Dysfunction in High-Fat Diet Fed Rodents. Scientific Reports, 2017, 7, 13523.	1.6	16

#	Article	IF	Citations
127	DI/LC-MS/MS-Based Metabolic Profiling for Identification of Early Predictive Serum Biomarkers of Metritis in Transition Dairy Cows. Journal of Agricultural and Food Chemistry, 2017, 65, 8510-8521.	2.4	20
128	Unraveling the meaning of chemical shifts in protein NMR. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2017, 1865, 1564-1576.	1.1	22
129	A Web Tool for Generating High Quality Machine-readable Biological Pathways. Journal of Visualized Experiments, 2017, , .	0.2	6
130	Metallotyping of ketotic dairy cows reveals major alterations preceding, associating, and following the disease occurrence. Metabolomics, 2017, 13, 1.	1.4	4
131	Initial Structural Models of the AÎ²42 Dimer from Replica Exchange Molecular Dynamics Simulations. ACS Omega, 2017, 2, 7621-7636.	1.6	10
132	Combining traditional dietary assessment methods with novel metabolomics techniques: present efforts by the Food Biomarker Alliance. Proceedings of the Nutrition Society, 2017, 76, 619-627.	0.4	93
133	GCâ€“MS Metabolomics Identifies Metabolite Alterations That Precede Subclinical Mastitis in the Blood of Transition Dairy Cows. Journal of Proteome Research, 2017, 16, 433-446.	1.8	72
134	Metabolomic determination of pathogenesis of late-onset preeclampsia. Journal of Maternal-Fetal and Neonatal Medicine, 2017, 30, 658-664.	0.7	35
135	The future of NMR-based metabolomics. Current Opinion in Biotechnology, 2017, 43, 34-40.	3.3	651
136	Dietary and health biomarkersâ€”time for an update. Genes and Nutrition, 2017, 12, 24.	1.2	43
137	A scheme for a flexible classification of dietary and health biomarkers. Genes and Nutrition, 2017, 12, 34.	1.2	76
138	Development and Validation of a High-Throughput Mass Spectrometry Based Urine Metabolomic Test for the Detection of Colonic Adenomatous Polyps. Metabolites, 2017, 7, 32.	1.3	30
139	YMDB 2.0: a significantly expanded version of the yeast metabolome database. Nucleic Acids Research, 2017, 45, D440-D445.	6.5	137
140	Livestock metabolomics and the livestock metabolome: A systematic review. PLoS ONE, 2017, 12, e0177675.	1.1	226
141	Dietary and metabolomic determinants of relapse in ulcerative colitis patients: A pilot prospective cohort study. World Journal of Gastroenterology, 2017, 23, 3890.	1.4	28
142	Cancer Metabolomics and the Human Metabolome Database. Metabolites, 2016, 6, 10.	1.3	116
143	Current and Future Perspectives on the Structural Identification of Small Molecules in Biological Systems. Metabolites, 2016, 6, 46.	1.3	110
144	Inter-Laboratory Robustness of Next-Generation Bile Acid Study in Mice and Humans: International Ring Trial Involving 12 Laboratories. journal of applied laboratory medicine, The, 2016, 1, 129-142.	0.6	30

#	Article	IF	Citations
145	Computational Prediction of Electron Ionization Mass Spectra to Assist in GC/MS Compound Identification. Analytical Chemistry, 2016, 88, 7689-7697.	3.2	109
146	Using DrugBank for In Silico Drug Exploration and Discovery. Current Protocols in Bioinformatics, 2016, 54, 14.4.1-14.4.31.	25.8	26
147	Role of polysaccharide and lipid in lipopolysaccharide induced prion protein conversion. Prion, 2016, 10, 466-483.	0.9	7
148	Live demonstration: Portable impedance-based biosensor system for metabolomic sensing. , 2016, , .		0
149	Heatmapper: web-enabled heat mapping for all. Nucleic Acids Research, 2016, 44, W147-W153.	6.5	1,766
150	Serum metabolomic markers for traumatic brain injury: a mouse model. Metabolomics, 2016, 12, 1.	1.4	22
151	Characterization of a highly potent antimicrobial peptide microcin N from uropathogenicEscherichia coli. FEMS Microbiology Letters, 2016, 363, fnw095.	0.7	13
152	Metabolomics enables precision medicine: â€œA White Paper, Community Perspectiveâ€• Metabolomics, 2016, 12, 149.	1.4	434
153	Using MetaboAnalyst 3.0 for Comprehensive Metabolomics Data Analysis. Current Protocols in Bioinformatics, 2016, 55, 14.10.1-14.10.91.	25.8	1,293
154	ClassyFire: automated chemical classification with a comprehensive, computable taxonomy. Journal of Cheminformatics, 2016, 8, 61.	2.8	779
155	Nano-Optomechanical Systems for Gas Chromatography. Nano Letters, 2016, 16, 6975-6981.	4.5	28
156	SPLASH, a hashed identifier for mass spectra. Nature Biotechnology, 2016, 34, 1099-1101.	9.4	61
157	An impedance detection circuit for applications in a portable biosensor system. , 2016, , .		6
158	PHASTER: a better, faster version of the PHAST phage search tool. Nucleic Acids Research, 2016, 44, W16-W21.	6.5	3,133
159	Metabolic signatures of Huntington's disease (HD): 1 H NMR analysis of the polar metabolome in post-mortem human brain. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2016, 1862, 1675-1684.	1.8	44
160	Introduction to Cheminformatics. Current Protocols in Bioinformatics, 2016, 53, 14.1.1-14.1.21.	25.8	15
161	Detecting Renal Allograft Inflammation Using Quantitative Urine Metabolomics and CXCL10. Transplantation Direct, 2016, 2, e78.	0.8	19
162	Clinical phenotype clustering in cardiovascular risk patients for the identification of responsive metabotypes after red wine polyphenol intake. Journal of Nutritional Biochemistry, 2016, 28, 114-120.	1.9	53

#	Article	IF	Citations
163	ECMDB 2.0: A richer resource for understanding the biochemistry ofE. coli. Nucleic Acids Research, 2016, 44, D495-D501.	6.5	121
164	Identification of candidate biomarkers of brain damage in a mouse model of closed head injury: a metabolomic pilot study. Metabolomics, 2016, 12, 1.	1.4	15
165	Emerging applications of metabolomics in drug discovery and precision medicine. Nature Reviews Drug Discovery, 2016, 15, 473-484.	21.5	1,029
166	Recommendations and Standardization of Biomarker Quantification Using NMR-Based Metabolomics with Particular Focus on Urinary Analysis. Journal of Proteome Research, 2016, 15, 360-373.	1.8	122
167	Isolation of soluble scFv antibody fragments specific for small biomarker molecule, L-Carnitine, using phage display. Journal of Immunological Methods, 2016, 428, 9-19.	0.6	7
168	Sildenafil Therapy Normalizes the Aberrant Metabolomic Profile in the Comtâ^'/â^' Mouse Model of Preeclampsia/Fetal Growth Restriction. Scientific Reports, 2015, 5, 18241.	1.6	26
169	Pathways with PathWhiz. Nucleic Acids Research, 2015, 43, W552-W559.	6.5	27
170	Defects in fatty acid amide hydrolase 2 in a male with neurologic and psychiatric symptoms. Orphanet Journal of Rare Diseases, 2015, 10, 38.	1.2	19
171	Metabolomics Approach Reveals Altered Plasma Amino Acid and Sphingolipid Profiles Associated with Pathololgical State in Transition Dairy Cows. Current Metabolomics, 2015, 2, 184-195.	0.5	23
172	Simulations of Interdigitated Electrode Interactions with Gold Nanoparticles for Impedance-Based Biosensing Applications. Sensors, 2015, 15, 22192-22208.	2.1	55
173	Accurate, Fully-Automated NMR Spectral Profiling for Metabolomics. PLoS ONE, 2015, 10, e0124219.	1.1	206
174	T3DB: the toxic exposome database. Nucleic Acids Research, 2015, 43, D928-D934.	6.5	228
175	MetaboAnalyst 3.0â€"making metabolomics more meaningful. Nucleic Acids Research, 2015, 43, W251-W257.	6.5	2,493
176	PolySearch2: a significantly improved text-mining system for discovering associations between human diseases, genes, drugs, metabolites, toxins and more. Nucleic Acids Research, 2015, 43, W535-W542.	6.5	143
177	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. Nature Structural and Molecular Biology, 2015, 22, 433-434.	3.6	40
178	CSI 3.0: a web server for identifying secondary and super-secondary structure in proteins using NMR chemical shifts. Nucleic Acids Research, 2015, 43, W370-W377.	6.5	128
179	Metabolome analysis of 20 taxonomically related benzylisoquinoline alkaloid-producing plants. BMC Plant Biology, 2015, 15, 220.	1.6	49
180	A robust algorithm for optimizing protein structures with NMR chemical shifts. Journal of Biomolecular NMR, 2015, 63, 255-264.	1.6	9

#	Article	IF	Citations
181	Standardizing the experimental conditions for using urine in NMR-based metabolomic studies with a particular focus on diagnostic studies: a review. Metabolomics, 2015, 11, 872-894.	1.4	196
182	Role of Water in Ligand Binding to Maltose-Binding Protein: Insight from a New Docking Protocol Based on the 3D-RISM-KH Molecular Theory of Solvation. Journal of Chemical Information and Modeling, 2015, 55, 317-328.	2.5	20
183	Recombinant mouse prion protein alone or in combination with lipopolysaccharide alters expression of innate immunity genes in the colon of mice. Prion, 2015, 9, 59-73.	0.9	6
184	Accessible surface area from NMR chemical shifts. Journal of Biomolecular NMR, 2015, 62, 387-401.	1.6	8
185	Is Cancer a Genetic Disease or a Metabolic Disease?. EBioMedicine, 2015, 2, 478-479.	2.7	110
186	Simulating electrical properties of interdigitated electrode designs for impedance-based biosensing applications. , 2015, , .		3
187	Validation of metabolomic models for prediction of early-onset preeclampsia. American Journal of Obstetrics and Gynecology, 2015, 213, 530.e1-530.e10.	0.7	51
188	The human saliva metabolome. Metabolomics, 2015, 11, 1864-1883.	1.4	195
189	Metabolite profiling and expression analysis of flavonoid, vitamin C and tocopherol biosynthesis genes in the antioxidant-rich sea buckthorn (Hippophae rhamnoides L.). Phytochemistry, 2015, 118, 181-191.	1.4	34
190	In silico studies and fluorescence binding assays of potential anti-prion compounds reveal an important binding site for prion inhibition from PrPC to PrPSc. European Journal of Medicinal Chemistry, 2015, 91, 118-131.	2.6	10
191	Salmonella Phages and Prophages: Genomics, Taxonomy, and Applied Aspects. Methods in Molecular Biology, 2015, 1225, 237-287.	0.4	31
192	Competitive fragmentation modeling of ESI-MS/MS spectra for putative metabolite identification. Metabolomics, 2015, 11, 98-110.	1.4	319
193	Metabolomic Fingerprint of Heart Failure with Preserved Ejection Fraction. PLoS ONE, 2015, 10, e0124844.	1.1	150
194	Identifying Putative Drug Targets and Potential Drug Leads: Starting Points for Virtual Screening and Docking. Methods in Molecular Biology, 2015, 1215, 425-444.	0.4	3
195	Shaking Alone Induces De Novo Conversion of Recombinant Prion Proteins to Î²-Sheet Rich Oligomers and Fibrils. PLoS ONE, 2014, 9, e98753.	1.1	33
196	pE-DB: a database of structural ensembles of intrinsically disordered and of unfolded proteins. Nucleic Acids Research, 2014, 42, D326-D335.	6.5	195
197	DrugBank 4.0: shedding new light on drug metabolism. Nucleic Acids Research, 2014, 42, D1091-D1097.	6.5	1,884
198	Lipopolysaccharide induced conversion of recombinant prion protein. Prion, 2014, 8, 221-232.	0.9	26

#	Article	IF	Citations
199	The Blood Exposome and Its Role in Discovering Causes of Disease. Environmental Health Perspectives, 2014, 122, 769-774.	2.8	283
200	CSI 2.0: a significantly improved version of the Chemical Shift Index. Journal of Biomolecular NMR, 2014, 60, 131-146.	1.6	47
201	Hair Metabolomics: Identification of Fetal Compromise Provides Proof of Concept for Biomarker Discovery. Theranostics, 2014, 4, 953-959.	4.6	68
202	CFM-ID: a web server for annotation, spectrum prediction and metabolite identification from tandem mass spectra. Nucleic Acids Research, 2014, 42, W94-W99.	6.5	369
203	A simple and sensitive biosensor for rapid detection of nanoparticles in water. Journal of Nanoparticle Research, 2014, 16, 1.	0.8	6
204	Metabolomic prediction of fetal congenital heart defect in the first trimester. American Journal of Obstetrics and Gynecology, 2014, 211, 240.e1-240.e14.	0.7	48
205	Brassica villosa, a system for studying non-glandular trichomes and genes in the Brassicas. Plant Molecular Biology, 2014, 85, 519-539.	2.0	25
206	Developing Trends in Aptamer-Based Biosensor Devices and Their Applications. IEEE Transactions on Biomedical Circuits and Systems, 2014, 8, 4-14.	2.7	38
207	The Use of Metabolomics in Population-Based Research. Advances in Nutrition, 2014, 5, 785-788.	2.9	18
208	SMPDB 2.0: Big Improvements to the Small Molecule Pathway Database. Nucleic Acids Research, 2014, 42, D478-D484.	6.5	341
209	The food metabolome: a window over dietary exposure. American Journal of Clinical Nutrition, 2014, 99, 1286-1308.	2.2	411
210	Development of Isotope Labeling Liquid Chromatography Mass Spectrometry for Mouse Urine Metabolomics: Quantitative Metabolomic Study of Transgenic Mice Related to Alzheimerâ€™s Disease. Journal of Proteome Research, 2014, 13, 4457-4469.	1.8	48
211	Using isotopically-coded hydrogen peroxide as a surface modification reagent for the structural characterization of prion protein aggregates. Journal of Proteomics, 2014, 100, 160-166.	1.2	10
212	Guest Editorialâ€"Special Issue on '-Omics' Based Companion Diagnostics for Personalized Medicine. IEEE Transactions on Biomedical Circuits and Systems, 2014, 8, 1-3.	2.7	4
213	Exploring the Human Metabolome by Nuclear Magnetic Resonance Spectroscopy and Mass Spectrometry. , 2013, , 3-29.		5
214	An improved method to detect correct protein folds using partial clustering. BMC Bioinformatics, 2013, 14, 11.	1.2	23
215	Experimental and Computational Study of the Interaction of Novel Colchicinoids with a Recombinant Human Î±<scp>I</scp>/Î²<scp>I</scp>â€Tubulin Heterodimer. Chemical Biology and Drug Design, 2013, 82, 60-70.	1.5	8
216	Characterization of biopharmaceuticals by NMR spectroscopy. TrAC - Trends in Analytical Chemistry, 2013, 48, 96-111.	5.8	37

#	Article	IF	Citations
217	Translational biomarker discovery in clinical metabolomics: an introductory tutorial. Metabolomics, 2013, 9, 280-299.	1.4	765
218	The Bovine Ruminal Fluid Metabolome. Metabolomics, 2013, 9, 360-378.	1.4	130
219	MyCompoundID: Using an Evidence-Based Metabolome Library for Metabolite Identification. Analytical Chemistry, 2013, 85, 3401-3408.	3.2	185
220	Molecular docking of thiamine reveals similarity in binding properties between the prion protein and other thiamine-binding proteins. Journal of Molecular Modeling, 2013, 19, 5225-5235.	0.8	12
221	A Simple Method to Measure Protein Side-Chain Mobility Using NMR Chemical Shifts. Journal of the American Chemical Society, 2013, 135, 14536-14539.	6.6	27
222	Using multiple structural proteomics approaches for the characterization of prion proteins. Journal of Proteomics, 2013, 81, 31-42.	1.2	18
223	Differential metabolite profiles and salinity tolerance between two genetically related brown-seeded and yellow-seeded Brassica carinata lines. Plant Science, 2013, 198, 17-26.	1.7	13
224	Metabolomic analysis for first-trimester trisomy 18 detection. American Journal of Obstetrics and Gynecology, 2013, 209, 65.e1-65.e9.	0.7	19
225	Recommendations of the wwPDB NMR Validation Task Force. Structure, 2013, 21, 1563-1570.	1.6	151
226	Metabolomic analysis for first-trimester Down syndrome prediction. American Journal of Obstetrics and Gynecology, 2013, 208, 371.e1-371.e8.	0.7	39
227	First-trimester metabolomic detection of late-onset preeclampsia. American Journal of Obstetrics and Gynecology, 2013, 208, 58.e1-58.e7.	0.7	60
228	Small Molecule Inhibitors of ERCC1-XPF Protein-Protein Interaction Synergize Alkylating Agents in Cancer Cells. Molecular Pharmacology, 2013, 84, 12-24.	1.0	80
229	The Human Urine Metabolome. PLoS ONE, 2013, 8, e73076.	1.1	1,125
230	Phenol-Explorer 3.0: a major update of the Phenol-Explorer database to incorporate data on the effects of food processing on polyphenol content. Database: the Journal of Biological Databases and Curation, 2013, 2013, bat070-bat070.	1.4	590
231	Identification and characterization of Ï•H111-1. Bacteriophage, 2013, 3, e26649.	1.9	5
232	INMEXâ€"a web-based tool for integrative meta-analysis of expression data. Nucleic Acids Research, 2013, 41, W63-W70.	6.5	162
233	Metabolomic Analysis of Cold Acclimation of Arctic Mesorhizobium sp. Strain N33. PLoS ONE, 2013, 8, e84801.	1.1	13
234	Nanopore Analysis of Wild-Type and Mutant Prion Protein (PrPC): Single Molecule Discrimination and PrPC Kinetics. PLoS ONE, 2013, 8, e54982.	1.1	14

#	Article	IF	Citations
235	Picornain 3C (human rhinovirus). , 2013, , 2402-2406.		0
236	DrugBank. , 2012, , 55-65.		6
237	Chapter 3: Small Molecules and Disease. PLoS Computational Biology, 2012, 8, e1002805.	1.5	28
238	Prediction of Skeletal Muscle and Fat Mass in Patients with Advanced Cancer Using a Metabolomic Approach. Journal of Nutrition, 2012, 142, 14-21.	1.3	28
239	ECMDB: The E. coli Metabolome Database. Nucleic Acids Research, 2012, 41, D625-D630.	6.5	122
240	METAGENassist: a comprehensive web server for comparative metagenomics. Nucleic Acids Research, 2012, 40, W88-W95.	6.5	345
241	Metabolomics and first-trimester prediction of early-onset preeclampsia. Journal of Maternal-Fetal and Neonatal Medicine, 2012, 25, 1840-1847.	0.7	101
242	BacMap: an up-to-date electronic atlas of annotated bacterial genomes. Nucleic Acids Research, 2012, 40, D599-D604.	6.5	19
243	Phenol-Explorer 2.0: a major update of the Phenol-Explorer database integrating data on polyphenol metabolism and pharmacokinetics in humans and experimental animals. Database: the Journal of Biological Databases and Curation, 2012, 2012, bas031-bas031.	1.4	135
244	3D-RISM-D<scp>ock</scp>: A New Fragment-Based Drug Design Protocol. Journal of Chemical Theory and Computation, 2012, 8, 3356-3372.	2.3	37
245	Virtual Screening and Biological Evaluation of Inhibitors Targeting the XPA-ERCC1 Interaction. PLoS ONE, 2012, 7, e51329.	1.1	60
246	Resolution-by-proxy: a simple measure for assessing and comparing the overall quality of NMR protein structures. Journal of Biomolecular NMR, 2012, 53, 167-180.	1.6	61
247	Development of Ecom₅₀ and Retention Index Models for Nontargeted Metabolomics: Identification of 1,3-Dicyclohexylurea in Human Serum by HPLC/Mass Spectrometry. Journal of Chemical Information and Modeling, 2012, 52, 1222-1237.	2.5	46
248	YMDB: the Yeast Metabolome Database. Nucleic Acids Research, 2012, 40, D815-D820.	6.5	162
249	HMDB 3.0â€"The Human Metabolome Database in 2013. Nucleic Acids Research, 2012, 41, D801-D807.	6.5	2,564
250	Use of Proteinase K Nonspecific Digestion for Selective and Comprehensive Identification of Interpeptide Cross-links: Application to Prion Proteins. Molecular and Cellular Proteomics, 2012, 11, M111.013524-1-M111.013524-13.	2.5	46
251	Shouldn't enantiomeric purity be included in the 'minimum information about a bioactive entity? Response from the MIABE group. Nature Reviews Drug Discovery, 2012, 11, 730-730.	21.5	0
252	MetaboAnalyst 2.0--a comprehensive server for metabolomic data analysis. Nucleic Acids Research, 2012, 40, W127-W133.	6.5	1,058

#	Article	IF	Citations
253	Multi-platform characterization of the human cerebrospinal fluid metabolome: a comprehensive and quantitative update. Genome Medicine, 2012, 4, 38.	3.6	113
254	Fatty Acid Composition of Developing Sea Buckthorn (Hippophae rhamnoides L.) Berry and the Transcriptome of the Mature Seed. PLoS ONE, 2012, 7, e34099.	1.1	117
255	Exploring the essential collective dynamics of interacting proteins: Application to prion protein dimers. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1847-1865.	1.5	14
256	Resolution-enhanced native acidic gel electrophoresis: A method for resolving, sizing, and quantifying prion protein oligomers. Analytical Biochemistry, 2012, 426, 54-62.	1.1	18
257	Progeny of tobacco mosaic virus-infected Nicotiana tabacum plants exhibit trans-generational changes in metabolic profiles. Biocatalysis and Agricultural Biotechnology, 2012, 1, 115-123.	1.5	19
258	Discovery of Small Molecule Inhibitors that Interact with Î³â€Tubulin. Chemical Biology and Drug Design, 2012, 79, 639-652.	1.5	33
259	Systems Biology Resources Arising from the Human Metabolome Project. , 2012, , 157-175.		9
260	The Metabolomic Profile of Umbilical Cord Blood in Neonatal Hypoxic Ischaemic Encephalopathy. PLoS ONE, 2012, 7, e50520.	1.1	84
261	3D-RISM-KH approach for biomolecular modelling at nanoscale: thermodynamics of fibril formation and beyond. Molecular Simulation, 2011, 37, 718-728.	0.9	16
262	DrugBank 3.0: a comprehensive resource for 'Omics' research on drugs. Nucleic Acids Research, 2011, 39, D1035-D1041.	6.5	1,566
263	Relative and Regional Stabilities of the Hamster, Mouse, Rabbit, and Bovine Prion Proteins toward Urea Unfolding Assessed by Nuclear Magnetic Resonance and Circular Dichroism Spectroscopies. Biochemistry, 2011, 50, 7536-7545.	1.2	22
264	Detailed Biophysical Characterization of the Acid-Induced PrP^c to PrP^{Î²} Conversion Process. Biochemistry, 2011, 50, 1162-1173.	1.2	85
265	Calculation of Local Water Densities in Biological Systems: A Comparison of Molecular Dynamics Simulations and the 3D-RISM-KH Molecular Theory of Solvation. Journal of Physical Chemistry B, 2011, 115, 319-328.	1.2	80
266	Metabolomic Data Processing, Analysis, and Interpretation Using MetaboAnalyst. Current Protocols in Bioinformatics, 2011, 34, Unit 14.10.	25.8	190
267	Molecular Signatures of End-Stage Heart Failure. Journal of Cardiac Failure, 2011, 17, 867-874.	0.7	30
268	Advances in metabolite identification. Bioanalysis, 2011, 3, 1769-1782.	0.6	238
269	Minimum information about a bioactive entity (MIABE). Nature Reviews Drug Discovery, 2011, 10, 661-669.	21.5	80
270	Databases on Food Phytochemicals and Their Health-Promoting Effects. Journal of Agricultural and Food Chemistry, 2011, 59, 4331-4348.	2.4	183

#	Article	IF	Citations
271	The Bacterial Nanorecorder: Engineering E. coli to Function as a Chemical Recording Device. PLoS ONE, 2011, 6, e27559.	1.1	8
272	The prion protein binds thiamine. FEBS Journal, 2011, 278, 4002-4014.	2.2	27
273	Web-based inference of biological patterns, functions and pathways from metabolomic data using MetaboAnalyst. Nature Protocols, 2011, 6, 743-760.	5.5	976
274	The Human Serum Metabolome. PLoS ONE, 2011, 6, e16957.	1.1	1,378
275	SHIFTX2: significantly improved protein chemical shift prediction. Journal of Biomolecular NMR, 2011, 50, 43-57.	1.6	575
276	Towards automatic metabolomic profiling of high-resolution one-dimensional proton NMR spectra. Journal of Biomolecular NMR, 2011, 49, 307-323.	1.6	117
277	Learning to predict cancer-associated skeletal muscle wasting from 1H-NMR profiles of urinary metabolites. Metabolomics, 2011, 7, 25-34.	1.4	51
278	Interpreting protein chemical shift data. Progress in Nuclear Magnetic Resonance Spectroscopy, 2011, 58, 62-87.	3.9	206
279	Comparative analysis of essential collective dynamics and NMR-derived flexibility profiles in evolutionarily diverse prion proteins. Prion, 2011, 5, 188-200.	0.9	22
280	PHAST: A Fast Phage Search Tool. Nucleic Acids Research, 2011, 39, W347-W352.	6.5	1,967
281	MetATT: a web-based metabolomics tool for analyzing time-series and two-factor datasets. Bioinformatics, 2011, 27, 2455-2456.	1.8	60
282	Intermolecular transmission of superoxide dismutase 1 misfolding in living cells. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 16398-16403.	3.3	234
283	Understanding Clostridium acetobutylicum ATCC 824 Metabolism Using Genome-Scale Thermodynamics and Metabolomics-based Modeling. IFAC Postprint Volumes IPPV / International Federation of Automatic Control, 2010, 43, 126-131.	0.4	2
284	A probabilistic approach for validating protein NMR chemical shift assignments. Journal of Biomolecular NMR, 2010, 47, 85-99.	1.6	34
285	Metabolomics reveals unhealthy alterations in rumen metabolism with increased proportion of cereal grain in the diet of dairy cows. Metabolomics, 2010, 6, 583-594.	1.4	174
286	Evidence for copurification of micronuclei in sucrose density gradient-enriched plasma membranes from cell lines. Analytical Biochemistry, 2010, 396, 69-75.	1.1	3
287	MSEA: a web-based tool to identify biologically meaningful patterns in quantitative metabolomic data. Nucleic Acids Research, 2010, 38, W71-W77.	6.5	582
288	PROSESS: a protein structure evaluation suite and server. Nucleic Acids Research, 2010, 38, W633-W640.	6.5	82

#	Article	IF	Citations
289	MetPA: a web-based metabolomics tool for pathway analysis and visualization. Bioinformatics, 2010, 26, 2342-2344.	1.8	624
290	T3DB: a comprehensively annotated database of common toxins and their targets. Nucleic Acids Research, 2010, 38, D781-D786.	6.5	126
291	SMPDB: The Small Molecule Pathway Database. Nucleic Acids Research, 2010, 38, D480-D487.	6.5	290
292	Computational Approaches to Metabolomics. Methods in Molecular Biology, 2010, 593, 283-313.	0.4	74
293	Association Thermodynamics and Conformational Stability of Î²-Sheet Amyloid Î²(17-42) Oligomers: Effects of E22Q (Dutch) Mutation and Charge Neutralization. Biophysical Journal, 2010, 98, 282-296.	0.2	49
294	Spatiotemporal integration of molecular and anatomical data in virtual reality using semantic mapping. International Journal of Nanomedicine, 2009, 4, 79.	3.3	4
295	Exploring Human Metabolites Using the Human Metabolome Database. Current Protocols in Bioinformatics, 2009, 25, Unit14.8.	25.8	38
296	Bioinformatics for Metabolomics. , 2009, , 581-599.		0
297	GeNMR: a web server for rapid NMR-based protein structure determination. Nucleic Acids Research, 2009, 37, W670-W677.	6.5	47
298	Mass-spectrometry-based metabolomics: limitations and recommendations for future progress with particular focus on nutrition research. Metabolomics, 2009, 5, 435-458.	1.4	462
299	Solid phase synthesis of acylglycine human metabolites. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 6706-6708.	1.0	2
300	HMDB: a knowledgebase for the human metabolome. Nucleic Acids Research, 2009, 37, D603-D610.	6.5	1,649
301	Essential Role of Hydration in Aggregation of Misfolded Prion Proteins: Quantification by Molecular Theory of Solvation. Journal of Toxicology and Environmental Health - Part A: Current Issues, 2009, 72, 1060-1068.	1.1	0
302	Development of a Novel Virtual Screening Cascade Protocol to Identify Potential Trypanothione Reductase Inhibitors. Journal of Medicinal Chemistry, 2009, 52, 1670-1680.	2.9	50
303	MetaboAnalyst: a web server for metabolomic data analysis and interpretation. Nucleic Acids Research, 2009, 37, W652-W660.	6.5	1,674
304	Computational strategies for metabolite identification in metabolomics. Bioanalysis, 2009, 1, 1579-1596.	0.6	103
305	In Sffamily Identification of Genes in Bacteriophage DNA. Methods in Molecular Biology, 2009, 502, 57-89.	0.4	25
306	Application of the random coil index to studying protein flexibility. Journal of Biomolecular NMR, 2008, 40, 31-48.	1.6	105

#	Article	IF	Citations
307	The human cerebrospinal fluid metabolome. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2008, 871, 164-173.	1.2	307
308	Liquid chromatography electrospray ionization and matrix-assisted laser desorption ionization tandem mass spectrometry for the analysis of lipid raft proteome of monocytes. Analytica Chimica Acta, 2008, 627, 82-90.	2.6	13
309	Quantitative metabolomics using NMR. TrAC - Trends in Analytical Chemistry, 2008, 27, 228-237.	5.8	484
310	Protein contact order prediction from primary sequences. BMC Bioinformatics, 2008, 9, 255.	1.2	19
311	MetaboMiner â€“ semi-automated identification of metabolites from 2D NMR spectra of complex biofluids. BMC Bioinformatics, 2008, 9, 507.	1.2	168
312	Genomic sequence and activity of KS10, a transposable phage of the Burkholderia cepacia complex. BMC Genomics, 2008, 9, 615.	1.2	27
313	Hydration Effects on the HET-s Prion and Amyloid-Î² Fibrillous Aggregates, Studied with Three-Dimensional Molecular Theory of Solvation. Biophysical Journal, 2008, 95, 4540-4548.	0.2	45
314	PSA fluoroimmunoassays using anti-PSA ScFv and quantum-dot conjugates. Nanomedicine, 2008, 3, 475-483.	1.7	14
315	Metabolomics: applications to food science and nutrition research. Trends in Food Science and Technology, 2008, 19, 482-493.	7.8	561
316	PolySearch: a web-based text mining system for extracting relationships between human diseases, genes, mutations, drugs and metabolites. Nucleic Acids Research, 2008, 36, W399-W405.	6.5	217
317	Applications of Metabolomics in DrugÂDiscovery and Development. Drugs in R and D, 2008, 9, 307-322.	1.1	174
318	DrugBank and its relevance to pharmacogenomics. Pharmacogenomics, 2008, 9, 1155-1162.	0.6	56
319	Metabolomics: A Complementary Tool in Renal Transplantation. , 2008, 160, 76-87.		36
320	CS23D: a web server for rapid protein structure generation using NMR chemical shifts and sequence data. Nucleic Acids Research, 2008, 36, W496-W502.	6.5	190
321	PROTEUS2: a web server for comprehensive protein structure prediction and structure-based annotation. Nucleic Acids Research, 2008, 36, W202-W209.	6.5	81
322	DrugBank: a knowledgebase for drugs, drug actions and drug targets. Nucleic Acids Research, 2008, 36, D901-D906.	6.5	2,336
323	Identifying Putative Drug Targets and Potential Drug Leads. Methods in Molecular Biology, 2008, 443, 333-351.	0.4	6
324	The RCI server: rapid and accurate calculation of protein flexibility using chemical shifts. Nucleic Acids Research, 2007, 35, W531-W537.	6.5	62

#	Article	IF	Citations
325	PPT-DB: the protein property prediction and testing database. Nucleic Acids Research, 2007, 36, D222-D229.	6.5	18
326	Human Metabolome Database: completing the â€˜human parts listâ€™. Pharmacogenomics, 2007, 8, 683-686.	0.6	44
327	Current Progress in computational metabolomics. Briefings in Bioinformatics, 2007, 8, 279-293.	3.2	185
328	Computational Systems Biology in Cancer: Modeling Methods and Applications. Gene Regulation and Systems Biology, 2007, 1, 117762500700100.	2.3	11
329	Discovering drug targets through the web. Comparative Biochemistry and Physiology Part D: Genomics and Proteomics, 2007, 2, 9-17.	0.4	9
330	HMDB: the Human Metabolome Database. Nucleic Acids Research, 2007, 35, D521-D526.	6.5	2,563
331	In Silico Drug Exploration and Discovery Using DrugBank. Current Protocols in Bioinformatics, 2007, 18, Unit 14.4.	25.8	6
332	Improving Early Drug Discovery through ADME Modelling. Drugs in R and D, 2007, 8, 349-362.	1.1	91
333	Proteomics and the Human Metabolome Project. Expert Review of Proteomics, 2007, 4, 333-335.	1.3	35
334	NMR Solution Structures of the Apo and Peptide-Inhibited Human Rhinovirus 3C Protease (Serotype 14):â€‰ Structural and Dynamic Comparison. Biochemistry, 2007, 46, 12945-12958.	1.2	27
335	Comparison of SDS- and methanol-assisted protein solubilization and digestion methods forEscherichia colimembrane proteome analysis by 2-D LC-MS/MS. Proteomics, 2007, 7, 484-493.	1.3	117
336	Computational systems biology in drug discovery and development: methods and applications. Drug Discovery Today, 2007, 12, 295-303.	3.2	132
337	Introduction to Cheminformatics. , 2007, Chapter 14, Unit 14.1.		17
338	Applications of machine learning in cancer prediction and prognosis. Cancer Informatics, 2007, 2, 59-77.	0.9	254
339	Computational systems biology in cancer: modeling methods and applications. Gene Regulation and Systems Biology, 2007, 1, 91-110.	2.3	27
340	Drug-target discovery in silico: using the web to identify novel molecular targets for drug action. SEB Experimental Biology Series, 2007, 58, 145-76.	0.1	1
341	BioSpider: a web server for automating metabolome annotations. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2007, , 145-56.	0.7	12
342	DrugBank: a comprehensive resource for in silico drug discovery and exploration. Nucleic Acids Research, 2006, 34, D668-D672.	6.5	3,070

#	Article	IF	Citations
343	Escherichia coli K-12: a cooperatively developed annotation snapshot--2005. Nucleic Acids Research, 2006, 34, 1-9.	6.5	606
344	Automated bacterial genome analysis and annotation. Current Opinion in Microbiology, 2006, 9, 505-510.	2.3	46
345	Applications of Machine Learning in Cancer Prediction and Prognosis. Cancer Informatics, 2006, 2, 117693510600200.	0.9	539
346	Metabolomics in monitoring kidney transplants. Current Opinion in Nephrology and Hypertension, 2006, 15, 637-642.	1.0	52
347	NMR: prediction of protein flexibility. Nature Protocols, 2006, 1, 683-688.	5.5	75
348	Improving the accuracy of protein secondary structure prediction using structural alignment. BMC Bioinformatics, 2006, 7, 301.	1.2	124
349	Accurate prediction of protein torsion angles using chemical shifts and sequence homology. Magnetic Resonance in Chemistry, 2006, 44, S158-S167.	1.1	43
350	PREDITOR: a web server for predicting protein torsion angle restraints. Nucleic Acids Research, 2006, 34, W63-W69.	6.5	171
351	Metabolomics: The Principles and Potential Applications to Transplantation. American Journal of Transplantation, 2005, 5, 2814-2820.	2.6	155
352	A simple method to adjust inconsistently referenced 13C and 15N chemical shift assignments of proteins. Journal of Biomolecular NMR, 2005, 31, 143-148.	1.6	32
353	Solution Structure of MTH0776 from Methanobacterium Thermoautotrophicum. Journal of Biomolecular NMR, 2005, 33, 51-56.	1.6	4
354	NMR Spectroscopy and Protein Structure Determination: Applications to Drug Discovery and Development. Current Pharmaceutical Biotechnology, 2005, 6, 105-120.	0.9	57
355	Identification of Novel and Known Oocyte-Specific Genes Using Complementary DNA Subtraction and Microarray Analysis in Three Different Species1. Biology of Reproduction, 2005, 73, 63-71.	1.2	61
356	MovieMaker: a web server for rapid rendering of protein motions and interactions. Nucleic Acids Research, 2005, 33, W358-W362.	6.5	46
357	Bioinformatics in Drug Development and Assessment. Drug Metabolism Reviews, 2005, 37, 279-310.	1.5	50
358	Circular genome visualization and exploration using CGView. Bioinformatics, 2005, 21, 537-539.	1.8	887
359	BASys: a web server for automated bacterial genome annotation. Nucleic Acids Research, 2005, 33, W455-W459.	6.5	290
360	A Simple Method To Predict Protein Flexibility Using Secondary Chemical Shifts. Journal of the American Chemical Society, 2005, 127, 14970-14971.	6.6	375

#	Article	IF	Citations
361	Bioinformatics in Drug Development and Assessment. Drug Metabolism Reviews, 2005, 37, 279-310.	1.5	13
362	Dynamic cellular automata: an alternative approach to cellular simulation. In Silico Biology, 2005, 5, 139-61.	0.4	27
363	SuperPose: a simple server for sophisticated structural superposition. Nucleic Acids Research, 2004, 32, W590-W594.	6.5	548
364	Proteome Analyst: custom predictions with explanations in a web-based tool for high-throughput proteome annotations. Nucleic Acids Research, 2004, 32, W365-W371.	6.5	93
365	PA-GOSUB: a searchable database of model organism protein sequences with their predicted Gene Ontology molecular function and subcellular localization. Nucleic Acids Research, 2004, 33, D147-D153.	6.5	23
366	GelScape: a web-based server for interactively annotating, manipulating, comparing and archiving 1D and 2D gel images. Bioinformatics, 2004, 20, 976-978.	1.8	21
367	The CyberCell Database (CCDB): a comprehensive, self-updating, relational database to coordinate and facilitate in silico modeling of Escherichia coli. Nucleic Acids Research, 2004, 32, 293D-295.	6.5	178
368	PlasMapper: a web server for drawing and auto-annotating plasmid maps. Nucleic Acids Research, 2004, 32, W660-W664.	6.5	68
369	NMR solution structure of the precursor for carnobacteriocin B2, an antimicrobial peptide from Carnobacterium piscicola. Implications of the alpha-helical leader section for export and inhibition of type IIa bacteriocin activity. FEBS Journal, 2004, 271, 1748-1756.	0.2	35
370	Solution structures of reduced and oxidized bacteriophage T4 glutaredoxin. Journal of Biomolecular NMR, 2004, 29, 85-90.	1.6	10
371	Letter to the Editor: Complete 1H, 13C and 15N NMR assignments of MTH0776 from Methanobacterium thermoautotrophicum. Journal of Biomolecular NMR, 2004, 30, 459-460.	1.6	1
372	Predictive Models for Breast Cancer Susceptibility from Multiple Single Nucleotide Polymorphisms. Clinical Cancer Research, 2004, 10, 2725-2737.	3.2	171
373	Identification of Bacteria Using Tandem Mass Spectrometry Combined with a Proteome Database and Statistical Scoring. Analytical Chemistry, 2004, 76, 2355-2366.	3.2	110
374	Synthesis and Evaluation of Keto-Glutamine Analogues as Potent Inhibitors of Severe Acute Respiratory Syndrome 3CLproâ€. Journal of Medicinal Chemistry, 2004, 47, 6113-6116.	2.9	98
375	Dynamic Relationships among Type IIa Bacteriocins:Â Temperature Effects on Antimicrobial Activity and on Structure of the C-Terminal Amphipathic Î± Helix as a Receptor-Binding Regionâ€¡. Biochemistry, 2004, 43, 9009-9020.	1.2	75
376	BacMap: an interactive picture atlas of annotated bacterial genomes. Nucleic Acids Research, 2004, 33, D317-D320.	6.5	48
377	Backbone 1H, 15N and 13C assignments for the human rhinovirus 3C protease (serotype 14). Journal of Biomolecular NMR, 2003, 26, 85-86.	1.6	2
378	Rapid and accurate calculation of protein 1H, 13C and 15N chemical shifts. Journal of Biomolecular NMR, 2003, 26, 215-240.	1.6	492

#	Article	IF	Citations
379	RefDB: a database of uniformly referenced protein chemical shifts. Journal of Biomolecular NMR, 2003, 25, 173-195.	1.6	391
380	Application of solid phase peptide synthesis to engineering PEOâ€“peptide block copolymers for drug delivery. Colloids and Surfaces B: Biointerfaces, 2003, 30, 323-334.	2.5	60
381	Structural and Functional Characterization of a Thioredoxin-Like Protein (Mt0807) from Methanobacterium thermoautotrophicum. Biochemistry, 2003, 42, 8001-8010.	1.2	11
382	VADAR: a web server for quantitative evaluation of protein structure quality. Nucleic Acids Research, 2003, 31, 3316-3319.	6.5	742
383	An NMR approach to structural proteomics. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 1825-1830.	3.3	195
384	Identification of a Novel Archaebacterial Thioredoxin:â€‰ Determination of Function through Structure. Biochemistry, 2002, 41, 4760-4770.	1.2	25
385	Use of Chemical Shifts in Macromolecular Structure Determination. Methods in Enzymology, 2002, 338, 3-34.	0.4	320
386	Probing the Structural Determinants of Type IIâ€˜ Î²-Turn Formation in Peptides and Proteins. Journal of the American Chemical Society, 2002, 124, 1203-1213.	6.6	93
387	Production of an Anti-Prostate-Specific Antigen Single-Chain Antibody Fragment from Pichia pastoris. Protein Expression and Purification, 2001, 23, 419-425.	0.6	13
388	Magnetic Resonance Diagnostics: A New Technology for High-Throughput Clinical Diagnostics. Clinical Chemistry, 2001, 47, 1918-1921.	1.5	25
389	Complete 1H, 13C and 15N backbone assignments for the hepatitis A virus 3C protease. Journal of Biomolecular NMR, 2001, 19, 187-188.	1.6	3
390	The BioTools Suite: A Comprehensive Suite of Platform-Independent Bioinformatics Tools. Molecular Biotechnology, 2001, 19, 059-078.	1.3	12
391	PepToolâ„¢ and GeneToolâ„¢: Platform-Independent Tools for Biological Sequence Analysis. , 2000, 132, 93-113.		21
392	Complete 1H and non-carbonylic 13C assignments of native hen egg-white lysozyme. Journal of Biomolecular NMR, 2000, 17, 83-84.	1.6	17
393	Analogues of Bacteriocins:â€‰ Antimicrobial Specificity and Interactions of Leucocin A with Its Enantiomer, Carnobacteriocin B2, and Truncated Derivatives. Journal of Medicinal Chemistry, 2000, 43, 4579-4581.	2.9	53
394	Solution Structure of Carnobacteriocin B2 and Implications for Structureâ^'Activity Relationships among Type IIa Bacteriocins from Lactic Acid Bacteriaâ€,â€¡. Biochemistry, 1999, 38, 15438-15447.	1.2	89
395	Facile measurement of polypeptide JHNH alpha coupling constants from HMQC-J spectra. , 1998, 11, 329-336.		6
396	CAMRA: chemical shift based computer aided protein NMR assignments. Journal of Biomolecular NMR, 1998, 12, 395-405.	1.6	46

#	Article	IF	Citations
397	Use of a Liposome Antigen Delivery System to Alter Immune Responses in Vivo. Journal of Pharmaceutical Sciences, 1998, 87, 1428-1432.	1.6	13
398	Unusual Î²-sheet periodicity in small cyclic peptides. Nature Structural Biology, 1998, 5, 284-288.	9.7	111
399	Protein chemical shift analysis: a practical guide. Biochemistry and Cell Biology, 1998, 76, 153-163.	0.9	176
400	A simple method to quantitatively measure polypeptide JHNH alpha coupling constants from TOCSY or NOESY spectra. Journal of Biomolecular NMR, 1997, 10, 373-382.	1.6	29
401	Automated 1H and 13C chemical shift prediction using the BioMagResBank. Journal of Biomolecular NMR, 1997, 10, 329-336.	1.6	85
402	ORB, a homology-based program for the prediction of protein NMR chemical shifts. Journal of Biomolecular NMR, 1997, 10, 165-179.	1.6	18
403	A method for the facile solid-phase synthesis of gramicidin S and its analogs. International Journal of Peptide Research and Therapeutics, 1996, 3, 53-60.	0.1	21
404	Peptide rescue of an Nâ€terminal truncation of the stoffel fragment of Taq DNA polymerase. Protein Science, 1996, 5, 1785-1792.	3.1	15
405	Modulation of Structure and Antibacterial and Hemolytic Activity by Ring Size in Cyclic Gramicidin S Analogs. Journal of Biological Chemistry, 1996, 271, 25261-25268.	1.6	172
406	Gramicidin S is active against both gramâ€positive and gramâ€negative bacteria. International Journal of Peptide and Protein Research, 1996, 47, 460-466.	0.1	149
407	On the Use of NMR in Complex Biological Systems: NMR Studies of Calcium Sensitive Interactions amongst Muscle Proteins. , 1996, , 275-284.		0
408	Vl-Linker-Vh Orientation-Dependent Expression of Single Chain Fv Containing an Engineered Disulfide-Stabilized Bond in the Framework Regions1. Journal of Biochemistry, 1995, 118, 825-831.	0.9	53
409	Design, synthesis and characterization of a water-soluble Î²-sheet peptide. Techniques in Protein Chemistry, 1995, 6, 451-457.	0.3	7
410	1H, 13C and 15N chemical shift referencing in biomolecular NMR. Journal of Biomolecular NMR, 1995, 6, 135-140.	1.6	2,216
411	1H, 13C and 15N random coil NMR chemical shifts of the common amino acids. I. Investigations of nearest-neighbor effects. Journal of Biomolecular NMR, 1995, 5, 67-81.	1.6	1,604
412	SEQSEE: a comprehensive program suite for protein sequence analysis. Bioinformatics, 1994, 10, 121-132.	1.8	40
413	Constrained multiple sequence alignment using XALIGN. Bioinformatics, 1994, 10, 687-688.	1.8	14
414	[12] Chemical shifts as a tool for structure determination. Methods in Enzymology, 1994, 239, 363-392.	0.4	803

#	Article	IF	Citations
415	Improved synthetic methods for the selective deuteration of aromatic amino acids: applications of selective protonation towards the identification of protein folding intermediates through nuclear magnetic resonance. BBA - Proteins and Proteomics, 1993, 1164, 36-46.	2.1	23
416	An improved synthesis of Î±-13C glycine and heteronuclear NMR studies of its incorporation into thioredoxin. Journal of Labelled Compounds and Radiopharmaceuticals, 1992, 31, 1019-1028.	0.5	3
417	Metabolomics in Humans and Other Mammals. , 0, , 253-288.		9
418	Proteins: Hormones, Enzymes, and Monoclonal Antibodiesâ€"Background. , 0, , 691-736.		1
419	The Childhood Acute Illness and Nutrition (CHAIN) network nested case-cohort study protocol: a multi-omics approach to understanding mortality among children in sub-Saharan Africa and South Asia. Gates Open Research, 0, 6, 77.	2.0	1