David Scott Wishart

List of Publications by Year
in descending order

419 papers	86,667 citations	1094 112 h-index	381 280 g-index
429 all docs	429 docs citations	429 times ranked	93996 citing authors

#	Article	IF	Citations
1	DrugBank 5.0: a major update to the DrugBank database for 2018. Nucleic Acids Research, 2018, 46, D1074-D1082.	6.5	5,428
2	MetaboAnalyst 4.0: towards more transparent and integrative metabolomics analysis. Nucleic Acids Research, 2018, 46, W486-W494.	6.5	3,199
3	PHASTER: a better, faster version of the PHAST phage search tool. Nucleic Acids Research, 2016, 44, W16-W21.	6.5	3,133
4	DrugBank: a comprehensive resource for in silico drug discovery and exploration. Nucleic Acids Research, 2006, 34, D668-D672.	6.5	3,070
5	HMDB 4.0: the human metabolome database for 2018. Nucleic Acids Research, 2018, 46, D608-D617.	6.5	2,805
6	HMDB 3.0â€”The Human Metabolome Database in 2013. Nucleic Acids Research, 2012, 41, D801-D807.	6.5	2,564
7	HMDB: the Human Metabolome Database. Nucleic Acids Research, 2007, 35, D521-D526.	6.5	2,563
8	MetaboAnalyst 3.0â€”making metabolomics more meaningful. Nucleic Acids Research, 2015, 43, W251-W257.	6.5	2,493
9	DrugBank: a knowledgebase for drugs, drug actions and drug targets. Nucleic Acids Research, 2008, 36, D901-D906.	6.5	2,336
10	1H, 13C and 15N chemical shift referencing in biomolecular NMR. Journal of Biomolecular NMR, 1995, 6, 135-140.	1.6	2,216
11	PHAST: A Fast Phage Search Tool. Nucleic Acids Research, 2011, 39, W347-W352.	6.5	1,967
12	DrugBank 4.0: shedding new light on drug metabolism. Nucleic Acids Research, 2014, 42, D1091-D1097.	6.5	1,884
13	Heatmapper: web-enabled heat mapping for all. Nucleic Acids Research, 2016, 44, W147-W153.	6.5	1,766
14	MetaboAnalyst: a web server for metabolomic data analysis and interpretation. Nucleic Acids Research, 2009, 37, W652-W660.	6.5	1,674
15	HMDB: a knowledgebase for the human metabolome. Nucleic Acids Research, 2009, 37, D603-D610.	6.5	1,649
16	Using MetaboAnalyst 4.0 for Comprehensive and Integrative Metabolomics Data Analysis. Current Protocols in Bioinformatics, 2019, 68, e86.	25.8	1,644
17	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
18	DrugBank 3.0: a comprehensive resource for 'Omics' research on drugs. Nucleic Acids Research, 2011, 39, D1035-D1041.	6.5	1,566

#	Article	IF	Citations
19	The Human Serum Metabolome. PLoS ONE, 2011, 6, e16957.	1.1	1,378
20	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
21	The Human Urine Metabolome. PLoS ONE, 2013, 8, e73076.	1.1	1,125
22	MetaboAnalyst 2.0--a comprehensive server for metabolomic data analysis. Nucleic Acids Research, 2012, 40, W127-W133.	6.5	1,058
23	Emerging applications of metabolomics in drug discovery and precision medicine. Nature Reviews Drug Discovery, 2016, 15, 473-484.	21.5	1,029
24	Web-based inference of biological patterns, functions and pathways from metabolomic data using MetaboAnalyst. Nature Protocols, 2011, 6, 743-760.	5.5	976
25	Circular genome visualization and exploration using CGView. Bioinformatics, 2005, 21, 537-539.	1.8	887
26	[12] Chemical shifts as a tool for structure determination. Methods in Enzymology, 1994, 239, 363-392.	0.4	803
27	ClassyFire: automated chemical classification with a comprehensive, computable taxonomy. Journal of Cheminformatics, 2016, 8, 61.	2.8	779
28	Translational biomarker discovery in clinical metabolomics: an introductory tutorial. Metabolomics, 2013, 9, 280-299.	1.4	765
29	VADAR: a web server for quantitative evaluation of protein structure quality. Nucleic Acids Research, 2003, 31, 3316-3319.	6.5	742
30	HMDB 5.0: the Human Metabolome Database for 2022. Nucleic Acids Research, 2022, 50, D622-D631.	6.5	736
31	The future of NMR-based metabolomics. Current Opinion in Biotechnology, 2017, 43, 34-40.	3.3	651
32	NMR Spectroscopy for Metabolomics Research. Metabolites, 2019, 9, 123.	1.3	627
33	MetPA: a web-based metabolomics tool for pathway analysis and visualization. Bioinformatics, 2010, 26, 2342-2344.	1.8	624
34	Escherichia coli K-12: a cooperatively developed annotation snapshot--2005. Nucleic Acids Research, 2006, 34, 1-9.	6.5	606
35	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
36	MSEA: a web-based tool to identify biologically meaningful patterns in quantitative metabolomic data. Nucleic Acids Research, 2010, 38, W71-W77.	6.5	582

#	Article	IF	Citations
37	SHIFTX2: significantly improved protein chemical shift prediction. Journal of Biomolecular NMR, 2011, 50, 43-57.	1.6	575
38	Metabolomics: applications to food science and nutrition research. Trends in Food Science and Technology, 2008, 19, 482-493.	7.8	561
39	SuperPose: a simple server for sophisticated structural superposition. Nucleic Acids Research, 2004, 32, W590-W594.	6.5	548
40	Applications of Machine Learning in Cancer Prediction and Prognosis. Cancer Informatics, 2006, 2, 117693510600200.	0.9	539
41	Metabolomics for Investigating Physiological and Pathophysiological Processes. Physiological Reviews, 2019, 99, 1819-1875.	13.1	516
42	Rapid and accurate calculation of protein 1H, 13C and 15N chemical shifts. Journal of Biomolecular NMR, 2003, 26, 215-240.	1.6	492
43	Quantitative metabolomics using NMR. TrAC - Trends in Analytical Chemistry, 2008, 27, 228-237.	5.8	484
44	Mass-spectrometry-based metabolomics: limitations and recommendations for future progress with particular focus on nutrition research. Metabolomics, 2009, 5, 435-458.	1.4	462
45	Metabolomics enables precision medicine: â€œA White Paper, Community Perspectiveâ€• Metabolomics, 2016, 12, 149.	1.4	434
46	The food metabolome: a window over dietary exposure. American Journal of Clinical Nutrition, 2014, 99, 1286-1308.	2.2	411
47	RefDB: a database of uniformly referenced protein chemical shifts. Journal of Biomolecular NMR, 2003, 25, 173-195.	1.6	391
48	Systems Biology and Multi-Omics Integration: Viewpoints from the Metabolomics Research Community. Metabolites, 2019, 9, 76.	1.3	387
49	A Simple Method To Predict Protein Flexibility Using Secondary Chemical Shifts. Journal of the American Chemical Society, 2005, 127, 14970-14971.	6.6	375
50	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
51	METAGENassist: a comprehensive web server for comparative metagenomics. Nucleic Acids Research, 2012, 40, W88-W95.	6.5	345
52	SMPDB 2.0: Big Improvements to the Small Molecule Pathway Database. Nucleic Acids Research, 2014, 42, D478-D484.	6.5	341
53	Use of Chemical Shifts in Macromolecular Structure Determination. Methods in Enzymology, 2002, 338, 3-34.	0.4	320
54	Competitive fragmentation modeling of ESI-MS/MS spectra for putative metabolite identification. Metabolomics, 2015, 11, 98-110.	1.4	319

#	Article	IF	Citations
55	The human cerebrospinal fluid metabolome. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2008, 871, 164-173.	1.2	307
56	BASys: a web server for automated bacterial genome annotation. Nucleic Acids Research, 2005, 33, W455-W459.	6.5	290
57	SMPDB: The Small Molecule Pathway Database. Nucleic Acids Research, 2010, 38, D480-D487.	6.5	290
58	The Blood Exposome and Its Role in Discovering Causes of Disease. Environmental Health Perspectives, 2014, 122, 769-774.	2.8	283
59	BioTransformer: a comprehensive computational tool for small molecule metabolism prediction and metabolite identification. Journal of Cheminformatics, 2019, 11, 2.	2.8	269
60	Applications of machine learning in cancer prediction and prognosis. Cancer Informatics, 2007, 2, 59-77.	0.9	254
61	Advances in metabolite identification. Bioanalysis, 2011, 3, 1769-1782.	0.6	238
62	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
63	T3DB: the toxic exposome database. Nucleic Acids Research, 2015, 43, D928-D934.	6.5	228
64	Livestock metabolomics and the livestock metabolome: A systematic review. PLoS ONE, 2017, 12, e0177675.	1.1	226
65	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
66	Interpreting protein chemical shift data. Progress in Nuclear Magnetic Resonance Spectroscopy, 2011, 58, 62-87.	3.9	206
67	Accurate, Fully-Automated NMR Spectral Profiling for Metabolomics. PLoS ONE, 2015, 10, e0124219.	1.1	206
68	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
69	CFM-ID 3.0: Significantly Improved ESI-MS/MS Prediction and Compound Identification. Metabolites, 2019, 9, 72.	1.3	196
70	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
71	pE-DB: a database of structural ensembles of intrinsically disordered and of unfolded proteins. Nucleic Acids Research, 2014, 42, D326-D335.	6.5	195
72	The human saliva metabolome. Metabolomics, 2015, 11, 1864-1883.	1.4	195

#	Article	IF	Citations
73	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
74	Metabolomic Data Processing, Analysis, and Interpretation Using MetaboAnalyst. Current Protocols in Bioinformatics, 2011, 34, Unit 14.10.	25.8	190
75	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
76	A review on human fecal metabolomics: Methods, applications and the human fecal metabolome database. Analytica Chimica Acta, 2018, 1030, 1-24.	2.6	187
77	Current Progress in computational metabolomics. Briefings in Bioinformatics, 2007, 8, 279-293.	3.2	185
78	MyCompoundID: Using an Evidence-Based Metabolome Library for Metabolite Identification. Analytical Chemistry, 2013, 85, 3401-3408.	3.2	185
79	Databases on Food Phytochemicals and Their Health-Promoting Effects. Journal of Agricultural and Food Chemistry, 2011, 59, 4331-4348.	2.4	183
80	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
81	Protein chemical shift analysis: a practical guide. Biochemistry and Cell Biology, 1998, 76, 153-163.	0.9	176
82	Applications of Metabolomics in DrugÂDiscovery and Development. Drugs in R and D, 2008, 9, 307-322.	1.1	174
83	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
84	Nutrimetabolomics: An Integrative Action for Metabolomic Analyses in Human Nutritional Studies. Molecular Nutrition and Food Research, 2019, 63, e1800384.	1.5	173
85	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
86	Predictive Models for Breast Cancer Susceptibility from Multiple Single Nucleotide Polymorphisms. Clinical Cancer Research, 2004, 10, 2725-2737.	3.2	171
87	PREDITOR: a web server for predicting protein torsion angle restraints. Nucleic Acids Research, 2006, 34, W63-W69.	6.5	171
88	MetaboMiner â€“ semi-automated identification of metabolites from 2D NMR spectra of complex biofluids. BMC Bioinformatics, 2008, 9, 507.	1.2	168
89	YMDB: the Yeast Metabolome Database. Nucleic Acids Research, 2012, 40, D815-D820.	6.5	162
90	INMEXâ€”a web-based tool for integrative meta-analysis of expression data. Nucleic Acids Research, 2013, 41, W63-W70.	6.5	162

#	Article	IF	Citations
91	Metabolomics: The Principles and Potential Applications to Transplantation. American Journal of Transplantation, 2005, 5, 2814-2820.	2.6	155
92	Recommendations of the wwPDB NMR Validation Task Force. Structure, 2013, 21, 1563-1570.	1.6	151
93	PHAST, PHASTER and PHASTEST: Tools for finding prophage in bacterial genomes. Briefings in Bioinformatics, 2019, 20, 1560-1567.	3.2	151
94	CFM-ID 4.0: More Accurate ESI-MS/MS Spectral Prediction and Compound Identification. Analytical Chemistry, 2021, 93, 11692-11700.	3.2	151
95	Metabolomic Fingerprint of Heart Failure with Preserved Ejection Fraction. PLoS ONE, 2015, 10, e0124844.	1.1	150
96	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
97	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
98	Chemical Composition of Commercial Cowâ€™s Milk. Journal of Agricultural and Food Chemistry, 2019, 67, 4897-4914.	2.4	139
99	YMDB 2.0: a significantly expanded version of the yeast metabolome database. Nucleic Acids Research, 2017, 45, D440-D445.	6.5	137
100	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
101	Computational systems biology in drug discovery and development: methods and applications. Drug Discovery Today, 2007, 12, 295-303.	3.2	132
102	The Bovine Ruminal Fluid Metabolome. Metabolomics, 2013, 9, 360-378.	1.4	130
103	NMR metabolomics: A look ahead. Journal of Magnetic Resonance, 2019, 306, 155-161.	1.2	129
104	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
105	T3DB: a comprehensively annotated database of common toxins and their targets. Nucleic Acids Research, 2010, 38, D781-D786.	6.5	126
106	Improving the accuracy of protein secondary structure prediction using structural alignment. BMC Bioinformatics, 2006, 7, 301.	1.2	124
107	ECMDB: The E. coli Metabolome Database. Nucleic Acids Research, 2012, 41, D625-D630.	6.5	122
108	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

#	Article	IF	Citations
109	ECMDB 2.0: A richer resource for understanding the biochemistry ofE. coli. Nucleic Acids Research, 2016, 44, D495-D501.	6.5	121
110	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
111	Towards automatic metabolomic profiling of high-resolution one-dimensional proton NMR spectra. Journal of Biomolecular NMR, 2011, 49, 307-323.	1.6	117
112	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
113	Cancer Metabolomics and the Human Metabolome Database. Metabolites, 2016, 6, 10.	1.3	116
114	Multi-platform characterization of the human cerebrospinal fluid metabolome: a comprehensive and quantitative update. Genome Medicine, 2012, 4, 38.	3.6	113
115	Unusual Î²-sheet periodicity in small cyclic peptides. Nature Structural Biology, 1998, 5, 284-288.	9.7	111
116	Identification of Bacteria Using Tandem Mass Spectrometry Combined with a Proteome Database and Statistical Scoring. Analytical Chemistry, 2004, 76, 2355-2366.	3.2	110
117	Is Cancer a Genetic Disease or a Metabolic Disease?. EBioMedicine, 2015, 2, 478-479.	2.7	110
118	Current and Future Perspectives on the Structural Identification of Small Molecules in Biological Systems. Metabolites, 2016, 6, 46.	1.3	110
119	Computational Prediction of Electron Ionization Mass Spectra to Assist in GC/MS Compound Identification. Analytical Chemistry, 2016, 88, 7689-7697.	3.2	109
120	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
121	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
122	Acylcarnitines: Nomenclature, Biomarkers, Therapeutic Potential, Drug Targets, and Clinical Trials. Pharmacological Reviews, 2022, 74, 506-551.	7.1	106
123	Application of the random coil index to studying protein flexibility. Journal of Biomolecular NMR, 2008, 40, 31-48.	1.6	105
124	CEU Mass Mediator 3.0: A Metabolite Annotation Tool. Journal of Proteome Research, 2019, 18, 797-802.	1.8	104
125	Computational strategies for metabolite identification in metabolomics. Bioanalysis, 2009, 1, 1579-1596.	0.6	103
126	Metabolomics and first-trimester prediction of early-onset preeclampsia. Journal of Maternal-Fetal and Neonatal Medicine, 2012, 25, 1840-1847.	0.7	101

#	Article	IF	Citations
127	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
128	Informatics and Data Analytics to Support Exposome-Based Discovery for Public Health. Annual Review of Public Health, 2017, 38, 279-294.	7.6	97
129	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
130	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
131	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
132	Metabolomics Profiling of Critically Ill Coronavirus Disease 2019 Patients: Identification of Diagnostic and Prognostic Biomarkers. , 2020, 2, e0272.		92
133	Improving Early Drug Discovery through ADME Modelling. Drugs in R and D, 2007, 8, 349-362.	1.1	91
134	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
135	Automated 1H and 13C chemical shift prediction using the BioMagResBank. Journal of Biomolecular NMR, 1997, 10, 329-336.	1.6	85
136	Detailed Biophysical Characterization of the Acid-Induced PrP^c to PrP^{Î²} Conversion Process. Biochemistry, 2011, 50, 1162-1173.	1.2	85
137	The Metabolomic Profile of Umbilical Cord Blood in Neonatal Hypoxic Ischaemic Encephalopathy. PLoS ONE, 2012, 7, e50520.	1.1	84
138	Microbiome and metabolome modifying effects of several cardiovascular disease interventions in apo-Eâ^'/â^' mice. Microbiome, 2017, 5, 30.	4.9	83
139	PathBank: a comprehensive pathway database for model organisms. Nucleic Acids Research, 2020, 48, D470-D478.	6.5	83
140	PROSESS: a protein structure evaluation suite and server. Nucleic Acids Research, 2010, 38, W633-W640.	6.5	82
141	PROTEUS2: a web server for comprehensive protein structure prediction and structure-based annotation. Nucleic Acids Research, 2008, 36, W202-W209.	6.5	81
142	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
143	Minimum information about a bioactive entity (MIABE). Nature Reviews Drug Discovery, 2011, 10, 661-669.	21.5	80
144	Small Molecule Inhibitors of ERCC1-XPF Protein-Protein Interaction Synergize Alkylating Agents in Cancer Cells. Molecular Pharmacology, 2013, 84, 12-24.	1.0	80

#	Article	IF	Citations
145	Perspective: Dietary Biomarkers of Intake and Exposureâ€"Exploration with Omics Approaches. Advances in Nutrition, 2020, 11, 200-215.	2.9	79
146	The Bovine Metabolome. Metabolites, 2020, 10, 233.	1.3	77
147	A scheme for a flexible classification of dietary and health biomarkers. Genes and Nutrition, 2017, 12, 34.	1.2	76
148	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
149	NMR: prediction of protein flexibility. Nature Protocols, 2006, 1, 683-688.	5.5	75
150	Computational Approaches to Metabolomics. Methods in Molecular Biology, 2010, 593, 283-313.	0.4	74
151	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
152	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
153	Pasture Feeding Changes the Bovine Rumen and Milk Metabolome. Metabolites, 2018, 8, 27.	1.3	70
154	PlasMapper: a web server for drawing and auto-annotating plasmid maps. Nucleic Acids Research, 2004, 32, W660-W664.	6.5	68
155	Hair Metabolomics: Identification of Fetal Compromise Provides Proof of Concept for Biomarker Discovery. Theranostics, 2014, 4, 953-959.	4.6	68
156	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
157	MarkerDB: an online database of molecular biomarkers. Nucleic Acids Research, 2021, 49, D1259-D1267.	6.5	64
158	The RCI server: rapid and accurate calculation of protein flexibility using chemical shifts. Nucleic Acids Research, 2007, 35, W531-W537.	6.5	62
159	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
160	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
161	SPLASH, a hashed identifier for mass spectra. Nature Biotechnology, 2016, 34, 1099-1101.	9.4	61
162	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

#	Article	IF	Citations
163	MetATT: a web-based metabolomics tool for analyzing time-series and two-factor datasets. Bioinformatics, 2011, 27, 2455-2456.	1.8	60
164	Virtual Screening and Biological Evaluation of Inhibitors Targeting the XPA-ERCC1 Interaction. PLoS ONE, 2012, 7, e51329.	1.1	60
165	First-trimester metabolomic detection of late-onset preeclampsia. American Journal of Obstetrics and Gynecology, 2013, 208, 58.e1-58.e7.	0.7	60
166	NMR Spectroscopy and Protein Structure Determination: Applications to Drug Discovery and Development. Current Pharmaceutical Biotechnology, 2005, 6, 105-120.	0.9	57
167	DrugBank and its relevance to pharmacogenomics. Pharmacogenomics, 2008, 9, 1155-1162.	0.6	56
168	Simulations of Interdigitated Electrode Interactions with Gold Nanoparticles for Impedance-Based Biosensing Applications. Sensors, 2015, 15, 22192-22208.	2.1	55
169	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
170	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
171	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
172	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
173	Metabolomics in monitoring kidney transplants. Current Opinion in Nephrology and Hypertension, 2006, 15, 637-642.	1.0	52
174	Learning to predict cancer-associated skeletal muscle wasting from 1H-NMR profiles of urinary metabolites. Metabolomics, 2011, 7, 25-34.	1.4	51
175	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
176	Bioinformatics in Drug Development and Assessment. Drug Metabolism Reviews, 2005, 37, 279-310.	1.5	50
177	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
178	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
179	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
180	Metabolome analysis of 20 taxonomically related benzylisoquinoline alkaloid-producing plants. BMC Plant Biology, 2015, 15, 220.	1.6	49

#	Article	IF	Citations
181	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
182	BacMap: an interactive picture atlas of annotated bacterial genomes. Nucleic Acids Research, 2004, 33, D317-D320.	6.5	48
183	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
184	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
185	Chemical language models enable navigation in sparsely populated chemical space. Nature Machine Intelligence, 2021, 3, 759-770.	8.3	48
186	GeNMR: a web server for rapid NMR-based protein structure determination. Nucleic Acids Research, 2009, 37, W670-W677.	6.5	47
187	CSI 2.0: a significantly improved version of the Chemical Shift Index. Journal of Biomolecular NMR, 2014, 60, 131-146.	1.6	47
188	CAMRA: chemical shift based computer aided protein NMR assignments. Journal of Biomolecular NMR, 1998, 12, 395-405.	1.6	46
189	MovieMaker: a web server for rapid rendering of protein motions and interactions. Nucleic Acids Research, 2005, 33, W358-W362.	6.5	46
190	Automated bacterial genome analysis and annotation. Current Opinion in Microbiology, 2006, 9, 505-510.	2.3	46
191	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
192	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
193	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
194	PAMDB: a comprehensive Pseudomonas aeruginosa metabolome database. Nucleic Acids Research, 2018, 46, D575-D580.	6.5	45
195	Human Metabolome Database: completing the â€˜human parts listâ€™. Pharmacogenomics, 2007, 8, 683-686.	0.6	44
196	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
197	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
198	Accurate prediction of protein torsion angles using chemical shifts and sequence homology. Magnetic Resonance in Chemistry, 2006, 44, S158-S167.	1.1	43

#	Article	IF	Citations
199	Dietary and health biomarkersâ€"time for an update. Genes and Nutrition, 2017, 12, 24.	1.2	43
200	Assessing the performance of genome-wide association studies for predicting disease risk. PLoS ONE, 2019, 14, e0220215.	1.1	43
201	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
202	Targeted metabolomics identifies high performing diagnostic and prognostic biomarkers for COVID-19. Scientific Reports, 2021, 11, 14732.	1.6	41
203	SEQSEE: a comprehensive program suite for protein sequence analysis. Bioinformatics, 1994, 10, 121-132.	1.8	40
204	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
205	Metabolomic analysis for first-trimester Down syndrome prediction. American Journal of Obstetrics and Gynecology, 2013, 208, 371.e1-371.e8.	0.7	39
206	Comprehensive Targeted Metabolomic Assay for Urine Analysis. Analytical Chemistry, 2020, 92, 10627-10634.	3.2	39
207	NP-MRD: the Natural Products Magnetic Resonance Database. Nucleic Acids Research, 2022, 50, D665-D677.	6.5	39
208	Exploring Human Metabolites Using the Human Metabolome Database. Current Protocols in Bioinformatics, 2009, 25, Unit14.8.	25.8	38
209	Developing Trends in Aptamer-Based Biosensor Devices and Their Applications. IEEE Transactions on Biomedical Circuits and Systems, 2014, 8, 4-14.	2.7	38
210	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
211	Characterization of biopharmaceuticals by NMR spectroscopy. TrAC - Trends in Analytical Chemistry, 2013, 48, 96-111.	5.8	37
212	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
213	A High-Performing Plasma Metabolite Panel for Early-Stage Lung Cancer Detection. Cancers, 2020, 12, 622.	1.7	37
214	Metabolomics: A Complementary Tool in Renal Transplantation. , 2008, 160, 76-87.		36
215	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
216	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

#	Article	IF	Citations
217	Proteomics and the Human Metabolome Project. Expert Review of Proteomics, 2007, 4, 333-335.	1.3	35
218	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
219	Metabolomic determination of pathogenesis of late-onset preeclampsia. Journal of Maternal-Fetal and Neonatal Medicine, 2017, 30, 658-664.	0.7	35
220	A probabilistic approach for validating protein NMR chemical shift assignments. Journal of Biomolecular NMR, 2010, 47, 85-99.	1.6	34
221	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
222	Metabolomics in Exercise and Sports: A Systematic Review. Sports Medicine, 2022, 52, 547-583.	3.1	34
223	Discovery of Small Molecule Inhibitors that Interact with Î³â€Tubulin. Chemical Biology and Drug Design, 2012, 79, 639-652.	1.5	33
224	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
225	BioTransformer 3.0â€"a web server for accurately predicting metabolic transformation products. Nucleic Acids Research, 2022, 50, W115-W123.	6.5	33
226	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
227	Transformation of polyphenols found in pigmented gluten-free flours during in vitro large intestinal fermentation. Food Chemistry, 2019, 298, 125068.	4.2	32
228	Salmonella Phages and Prophages: Genomics, Taxonomy, and Applied Aspects. Methods in Molecular Biology, 2015, 1225, 237-287.	0.4	31
229	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
230	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
231	Molecular Signatures of End-Stage Heart Failure. Journal of Cardiac Failure, 2011, 17, 867-874.	0.7	30
232	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
233	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
234	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

#	Article	IF	Citations
235	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
236	Chapter 3: Small Molecules and Disease. PLoS Computational Biology, 2012, 8, e1002805.	1.5	28
237	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
238	Nano-Optomechanical Systems for Gas Chromatography. Nano Letters, 2016, 16, 6975-6981.	4.5	28
239	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
240	A deep generative model enables automated structure elucidation of novel psychoactive substances. Nature Machine Intelligence, 2021, 3, 973-984.	8.3	28
241	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
242	Genomic sequence and activity of KS10, a transposable phage of the Burkholderia cepacia complex. BMC Genomics, 2008, 9, 615.	1.2	27
243	The prion protein binds thiamine. FEBS Journal, 2011, 278, 4002-4014.	2.2	27
244	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
245	Pathways with PathWhiz. Nucleic Acids Research, 2015, 43, W552-W559.	6.5	27
246	Computational systems biology in cancer: modeling methods and applications. Gene Regulation and Systems Biology, 2007, 1, 91-110.	2.3	27
247	Dynamic cellular automata: an alternative approach to cellular simulation. In Silico Biology, 2005, 5, 139-61.	0.4	27
248	Lipopolysaccharide induced conversion of recombinant prion protein. Prion, 2014, 8, 221-232.	0.9	26
249	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
250	Using DrugBank for In Silico Drug Exploration and Discovery. Current Protocols in Bioinformatics, 2016, 54, 14.4.1-14.4.31.	25.8	26
251	Urinary Metabolomics for Noninvasive Detection of Antibody-Mediated Rejection in Children After Kidney Transplantation. Transplantation, 2017, 101, 2553-2561.	0.5	26
252	Metabolomic profiling of the excretoryâ€“secretory products of hookworm and whipworm. Metabolomics, 2019, 15, 101.	1.4	26

#	Article	IF	Citations
253	Magnetic Resonance Diagnostics: A New Technology for High-Throughput Clinical Diagnostics. Clinical Chemistry, 2001, 47, 1918-1921.	1.5	25
254	Identification of a Novel Archaebacterial Thioredoxin:â€‰ Determination of Function through Structure. Biochemistry, 2002, 41, 4760-4770.	1.2	25
255	Brassica villosa, a system for studying non-glandular trichomes and genes in the Brassicas. Plant Molecular Biology, 2014, 85, 519-539.	2.0	25
256	In Sffamily Identification of Genes in Bacteriophage DNA. Methods in Molecular Biology, 2009, 502, 57-89.	0.4	25
257	Metabolomic prediction of endometrial cancer. Metabolomics, 2018, 14, 6.	1.4	24
258	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
259	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
260	An improved method to detect correct protein folds using partial clustering. BMC Bioinformatics, 2013, 14, 11.	1.2	23
261	Metabolomics Approach Reveals Altered Plasma Amino Acid and Sphingolipid Profiles Associated with Patholological State in Transition Dairy Cows. Current Metabolomics, 2015, 2, 184-195.	0.5	23
262	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
263	Comparative analysis of essential collective dynamics and NMR-derived flexibility profiles in evolutionarily diverse prion proteins. Prion, 2011, 5, 188-200.	0.9	22
264	Serum metabolomic markers for traumatic brain injury: a mouse model. Metabolomics, 2016, 12, 1.	1.4	22
265	Unraveling the meaning of chemical shifts in protein NMR. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2017, 1865, 1564-1576.	1.1	22
266	Immunometabolic signatures predict risk of progression to sepsis in COVID-19. PLoS ONE, 2021, 16, e0256784.	1.1	22
267	Emerging technologies and their impact on regulatory science. Experimental Biology and Medicine, 2022, 247, 1-75.	1.1	22
268	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
269	PepToolâ„¢ and GeneToolâ„¢: Platform-Independent Tools for Biological Sequence Analysis. , 2000, 132, 93-113.		21
270	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

#	Article	IF	Citations
271	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
272	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
273	Impact of Bovine Diet on Metabolomic Profile of Skim Milk and Whey Protein Ingredients. Metabolites, 2019, 9, 305.	1.3	20
274	The Urinary Metabolome of Healthy Newborns. Metabolites, 2020, 10, 165.	1.3	20
275	Protein contact order prediction from primary sequences. BMC Bioinformatics, 2008, 9, 255.	1.2	19
276	BacMap: an up-to-date electronic atlas of annotated bacterial genomes. Nucleic Acids Research, 2012, 40, D599-D604.	6.5	19
277	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
278	Metabolomic analysis for first-trimester trisomy 18 detection. American Journal of Obstetrics and Gynecology, 2013, 209, 65.e1-65.e9.	0.7	19
279	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
280	Detecting Renal Allograft Inflammation Using Quantitative Urine Metabolomics and CXCL10. Transplantation Direct, 2016, 2, e78.	0.8	19
281	Candidate serum metabolite biomarkers of residual feed intake and carcass merit in sheep. Journal of Animal Science, 2020, 98, .	0.2	19
282	ORB, a homology-based program for the prediction of protein NMR chemical shifts. Journal of Biomolecular NMR, 1997, 10, 165-179.	1.6	18
283	PPT-DB: the protein property prediction and testing database. Nucleic Acids Research, 2007, 36, D222-D229.	6.5	18
284	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
285	Using multiple structural proteomics approaches for the characterization of prion proteins. Journal of Proteomics, 2013, 81, 31-42.	1.2	18
286	The Use of Metabolomics in Population-Based Research. Advances in Nutrition, 2014, 5, 785-788.	2.9	18
287	Serum Metabolite Biomarkers for Predicting Residual Feed Intake (RFI) of Young Angus Bulls. Metabolites, 2020, 10, 491.	1.3	18
288	Complete 1H and non-carbonylic 13C assignments of native hen egg-white lysozyme. Journal of Biomolecular NMR, 2000, 17, 83-84.	1.6	17

#	Article	IF	Citations
289	Introduction to Cheminformatics. , 2007, Chapter 14, Unit 14.1.		17
290	Metabolomics and the Multi-Omics View of Cancer. Metabolites, 2022, 12, 154.	1.3	17
291	3D-RISM-KH approach for biomolecular modelling at nanoscale: thermodynamics of fibril formation and beyond. Molecular Simulation, 2011, 37, 718-728.	0.9	16
292	Recombinant Incretin-Secreting Microbe Improves Metabolic Dysfunction in High-Fat Diet Fed Rodents. Scientific Reports, 2017, 7, 13523.	1.6	16
293	Peptide rescue of an Nâ€terminal truncation of the stoffel fragment of Taq DNA polymerase. Protein Science, 1996, 5, 1785-1792.	3.1	15
294	Introduction to Cheminformatics. Current Protocols in Bioinformatics, 2016, 53, 14.1.1-14.1.21.	25.8	15
295	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
296	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
297	The role of the Human Metabolome Database in inborn errors of metabolism. Journal of Inherited Metabolic Disease, 2018, 41, 329-336.	1.7	15
298	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
299	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
300	Targeted metabolomics highlights perturbed metabolism in the brain of autism spectrum disorder sufferers. Metabolomics, 2020, 16, 59.	1.4	15
301	A Comprehensive Targeted Metabolomics Assay for Crop Plant Sample Analysis. Metabolites, 2021, 11, 303.	1.3	15
302	Constrained multiple sequence alignment using XALIGN. Bioinformatics, 1994, 10, 687-688.	1.8	14
303	PSA fluoroimmunoassays using anti-PSA ScFv and quantum-dot conjugates. Nanomedicine, 2008, 3, 475-483.	1.7	14
304	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
305	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
306	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
307	Systemic inflammation and metabolic disturbances underlie inpatient mortality among ill children with severe malnutrition. Science Advances, 2022, 8, eabj6779.	4.7	14
308	Use of a Liposome Antigen Delivery System to Alter Immune Responses in Vivo. Journal of Pharmaceutical Sciences, 1998, 87, 1428-1432.	1.6	13
309	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
310	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
311	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
312	Metabolomic Analysis of Cold Acclimation of Arctic Mesorhizobium sp. Strain N33. PLoS ONE, 2013, 8, e84801.	1.1	13
313	Characterization of a highly potent antimicrobial peptide microcin N from uropathogenicEscherichia coli. FEMS Microbiology Letters, 2016, 363, fnw095.	0.7	13
314	Nonâ€invasive staging of chronic kidney allograft damage using urine metabolomic profiling. Pediatric Transplantation, 2018, 22, e13226.	0.5	13
315	Bioinformatics in Drug Development and Assessment. Drug Metabolism Reviews, 2005, 37, 279-310.	1.5	13
316	The BioTools Suite: A Comprehensive Suite of Platform-Independent Bioinformatics Tools. Molecular Biotechnology, 2001, 19, 059-078.	1.3	12
317	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
318	Non-invasive Point-of-Care Device To Diagnose Acute Mesenteric Ischemia. ACS Sensors, 2018, 3, 2296-2302.	4.0	12
319	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
320	Gut Microenvironment and Bacterial Invasion in Paediatric Inflammatory Bowel Diseases. Journal of Pediatric Gastroenterology and Nutrition, 2020, 71, 624-632.	0.9	12
321	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
322	Excretory/Secretory Metabolome of the Zoonotic Roundworm Parasite Toxocara canis. Biomolecules, 2020, 10, 1157.	1.8	12
323	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
324	BioSpider: a web server for automating metabolome annotations. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2007, , 145-56.	0.7	12

#	Article	IF	Citations
325	Structural and Functional Characterization of a Thioredoxin-Like Protein (Mt0807) from Methanobacterium thermoautotrophicum. Biochemistry, 2003, 42, 8001-8010.	1.2	11
326	Computational Systems Biology in Cancer: Modeling Methods and Applications. Gene Regulation and Systems Biology, 2007, 1, 117762500700100.	2.3	11
327	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
328	Solution structures of reduced and oxidized bacteriophage T4 glutaredoxin. Journal of Biomolecular NMR, 2004, 29, 85-90.	1.6	10
329	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
330	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
331	Initial Structural Models of the AÎ²42 Dimer from Replica Exchange Molecular Dynamics Simulations. ACS Omega, 2017, 2, 7621-7636.	1.6	10
332	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
333	A fast, sensitive, single-step colorimetric dipstick assay for quantifying ascorbic acid in urine. Analytical Biochemistry, 2019, 580, 1-13.	1.1	10
334	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
335	Discovering drug targets through the web. Comparative Biochemistry and Physiology Part D: Genomics and Proteomics, 2007, 2, 9-17.	0.4	9
336	Metabolomics in Humans and Other Mammals. , 0, , 253-288.		9
337	A robust algorithm for optimizing protein structures with NMR chemical shifts. Journal of Biomolecular NMR, 2015, 63, 255-264.	1.6	9
338	Urinary Metabolomics around Parturition Identifies Metabolite Alterations in Dairy Cows Affected Postpartum by Lameness: Preliminary Study. Dairy, 2020, 1, 2.	0.7	9
339	Systems Biology Resources Arising from the Human Metabolome Project. , 2012, , 157-175.		9
340	Automated Tools for the Analysis of 1D-NMR and 2D-NMR Spectra. Methods in Molecular Biology, 2019, 2037, 429-449.	0.4	9
341	Advances in Metabolomics-Driven Diagnostic Breeding and Crop Improvement. Metabolites, 2022, 12, 511.	1.3	9
342	The Bacterial Nanorecorder: Engineering E. coli to Function as a Chemical Recording Device. PLoS ONE, 2011, 6, e27559.	1.1	8

#	Article	IF	Citations
343	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
344	Accessible surface area from NMR chemical shifts. Journal of Biomolecular NMR, 2015, 62, 387-401.	1.6	8
345	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
346	Protocols for NMR Analysis in Livestock Metabolomics. Methods in Molecular Biology, 2019, 1996, 311-324.	0.4	8
347	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
348	Effect of Diet on the Vitamin B Profile of Bovine Milk-Based Protein Ingredients. Foods, 2020, 9, 578.	1.9	8
349	Design, synthesis and characterization of a water-soluble Î²-sheet peptide. Techniques in Protein Chemistry, 1995, 6, 451-457.	0.3	7
350	Role of polysaccharide and lipid in lipopolysaccharide induced prion protein conversion. Prion, 2016, 10, 466-483.	0.9	7
351	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
352	Facile measurement of polypeptide JHNH alpha coupling constants from HMQC-J spectra. , 1998, 11, 329-336.		6
353	In Silico Drug Exploration and Discovery Using DrugBank. Current Protocols in Bioinformatics, 2007, 18, Unit 14.4.	25.8	6
354	DrugBank. , 2012, , 55-65.		6
355	A simple and sensitive biosensor for rapid detection of nanoparticles in water. Journal of Nanoparticle Research, 2014, 16, 1.	0.8	6
356	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
357	An impedance detection circuit for applications in a portable biosensor system. , 2016, , .		6
358	A Web Tool for Generating High Quality Machine-readable Biological Pathways. Journal of Visualized Experiments, 2017, , .	0.2	6
359	Nonâ€invasive differentiation of nonâ€rejection kidney injury from acute rejection in pediatric renal transplant recipients. Pediatric Transplantation, 2019, 23, e13364.	0.5	6
360	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

#	Article	IF	Citations
361	Serum metabolomics identifies metabolite panels that differentiate lame dairy cows from healthy ones. Metabolomics, 2020, 16, 73.	1.4	6
362	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
363	Metabolomic Data Exploration and Analysis with the Human Metabolome Database. Methods in Molecular Biology, 2020, 2104, 165-184.	0.4	6
364	Identifying Putative Drug Targets and Potential Drug Leads. Methods in Molecular Biology, 2008, 443, 333-351.	0.4	6
365	Exploring the Human Metabolome by Nuclear Magnetic Resonance Spectroscopy and Mass Spectrometry. , 2013, , 3-29.		5
366	Identification and characterization of Ï•H111-1. Bacteriophage, 2013, 3, e26649.	1.9	5
367	Preparation and characterization of a highly soluble AÎ²1-42 peptide variant. Protein Expression and Purification, 2019, 164, 105480.	0.6	5
368	Porous Nanophotonic Optomechanical Beams for Enhanced Mass Adsorption. ACS Sensors, 2019, 4, 1197-1202.	4.0	5
369	First-trimester metabolomic prediction of stillbirth. Journal of Maternal-Fetal and Neonatal Medicine, 2019, 32, 3435-3441.	0.7	5
370	Value-based healthcare delivery through metabolomics-based personalized health platform. Healthcare Management Forum, 2020, 33, 126-134.	0.6	5
371	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
372	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
373	Solution Structure of MTH0776 from Methanobacterium Thermoautotrophicum. Journal of Biomolecular NMR, 2005, 33, 51-56.	1.6	4
374	Spatiotemporal integration of molecular and anatomical data in virtual reality using semantic mapping. International Journal of Nanomedicine, 2009, 4, 79.	3.3	4
375	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
376	Peptide-based fluorescence biosensors for detection/measurement of nanoparticles. Analytical and Bioanalytical Chemistry, 2017, 409, 903-915.	1.9	4
377	Metallotyping of ketotic dairy cows reveals major alterations preceding, associating, and following the disease occurrence. Metabolomics, 2017, 13, 1.	1.4	4
378	Rapid and reliable protein structure determination via chemical shift threading. Journal of Biomolecular NMR, 2018, 70, 33-51.	1.6	4

#	Article	IF	Citations
379	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
380	Urinary metabolomics to develop predictors for pediatric acute kidney injury. Pediatric Nephrology, 2022, 37, 2079-2090.	0.9	4
381	Predictive blood biomarkers of sheep pregnancy and litter size. Scientific Reports, 2022, 12, .	1.6	4
382	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
383	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
384	Evidence for copurification of micronuclei in sucrose density gradient-enriched plasma membranes from cell lines. Analytical Biochemistry, 2010, 396, 69-75.	1.1	3
385	Simulating electrical properties of interdigitated electrode designs for impedance-based biosensing applications. , 2015, , .		3
386	CpG-ODN induced antimicrobial immunity in neonatal chicks involves a substantial shift in serum metabolic profiles. Scientific Reports, 2021, 11, 9028.	1.6	3
387	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
388	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
389	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
390	Solid phase synthesis of acylglycine human metabolites. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 6706-6708.	1.0	2
391	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
392	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
393	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
394	Growth of Malignant Non-CNS Tumors Alters Brain Metabolome. Frontiers in Genetics, 2018, 9, 41.	1.1	2
395	Food Constituent and Food Metabolite Databases. , 2021, , 2-18.		2
396	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

#	Article	IF	Citations
397	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
398	Metabolomic Fingerprint of Behavioral Changes in Response to Full-Spectrum Cannabis Extracts. Frontiers in Pharmacology, 2022, 13, 831052.	1.6	2
399	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
400	Proteins: Hormones, Enzymes, and Monoclonal Antibodiesâ€"Background. , 0, , 691-736.		1
401	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
402	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
403	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
404	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
405	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
406	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
407	Bioinformatics for Metabolomics. , 2009, , 581-599.		0
408	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
409	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
410	Live demonstration: Portable impedance-based biosensor system for metabolomic sensing. , 2016, , .		0
411	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
412	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
413	Picornain 3C (human rhinovirus). , 2013, , 2402-2406.		0
414	On the Use of NMR in Complex Biological Systems: NMR Studies of Calcium Sensitive Interactions amongst Muscle Proteins. , 1996, , 275-284.		0

#	Article	IF	Citations
415	Assessing the performance of genome-wide association studies for predicting disease risk. , 2019, 14, e0220215.		0
416	Assessing the performance of genome-wide association studies for predicting disease risk. , 2019, 14, e0220215.		0
417	Assessing the performance of genome-wide association studies for predicting disease risk. , 2019, 14, e0220215.		0
418	Assessing the performance of genome-wide association studies for predicting disease risk. , 2019, 14, e0220215.		0
419	The impact of methodological choices when developing predictive models using urinary metabolite data. Statistics in Medicine, 2022, , .	0.8	0