David Scott Wishart

List of Publications by Citations

410 papers	62,704 citations	100 h-index	248 g-index
429 ext. papers	77,013 ext. citations	8.1 avg, IF	8.29 L-index

#	Paper	IF	Citations
410	DrugBank 5.0: a major update to the DrugBank database for 2018. *Nucleic Acids Research*, **2018**, 46, D1074-D1082	20.1	2762
409	DrugBank: a comprehensive resource for in silico drug discovery and exploration. *Nucleic Acids Research*, **2006**, 34, D668-72	20.1	2266
408	HMDB 3.0--The Human Metabolome Database in 2013. *Nucleic Acids Research*, **2013**, 41, D801-7	20.1	2210
407	MetaboAnalyst 4.0: towards more transparent and integrative metabolomics analysis. *Nucleic Acids Research*, **2018**, 46, W486-W494	20.1	2157
406	MetaboAnalyst 3.0--making metabolomics more meaningful. *Nucleic Acids Research*, **2015**, 43, W251-7	20.1	2067
405	1H, 13C and 15N chemical shift referencing in biomolecular NMR. *Journal of Biomolecular NMR*, **1995**, 6, 135-40	3	2054
404	HMDB: the Human Metabolome Database. *Nucleic Acids Research*, **2007**, 35, D521-6	20.1	2021
403	HMDB 4.0: the human metabolome database for 2018. *Nucleic Acids Research*, **2018**, 46, D608-D617	20.1	1832
402	DrugBank: a knowledgebase for drugs, drug actions and drug targets. *Nucleic Acids Research*, **2008**, 36, D901-6	20.1	1770
401	PHASTER: a better, faster version of the PHAST phage search tool. *Nucleic Acids Research*, **2016**, 44, W16-21	20.1	1573
400	DrugBank 4.0: shedding new light on drug metabolism. *Nucleic Acids Research*, **2014**, 42, D1091-7	20.1	1490
399	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	3	1487
398	HMDB: a knowledgebase for the human metabolome. *Nucleic Acids Research*, **2009**, 37, D603-10	20.1	1431
397	PHAST: a fast phage search tool. *Nucleic Acids Research*, **2011**, 39, W347-52	20.1	1392
396	DrugBank 3.0: a comprehensive resource for 'Omics' research on drugs. *Nucleic Acids Research*, **2011**, 39, D1035-41	20.1	1355
395	MetaboAnalyst: a web server for metabolomic data analysis and interpretation. *Nucleic Acids Research*, **2009**, 37, W652-60	20.1	1202
394	The human serum metabolome. *PLoS ONE*, **2011**, 6, e16957	3.7	1118

393	Heatmapper: web-enabled heat mapping for all. *Nucleic Acids Research*, **2016**, 44, W147-53	20.1	957
392	Using MetaboAnalyst 3.0 for Comprehensive Metabolomics Data Analysis. *Current Protocols in Bioinformatics*, **2016**, 55, 14.10.1-14.10.91	24.2	957
391	MetaboAnalyst 2.0--a comprehensive server for metabolomic data analysis. *Nucleic Acids Research*, **2012**, 40, W127-33	20.1	935
390	Using MetaboAnalyst 4.0 for Comprehensive and Integrative Metabolomics Data Analysis. *Current Protocols in Bioinformatics*, **2019**, 68, e86	24.2	928
389	The human urine metabolome. *PLoS ONE*, **2013**, 8, e73076	3.7	862
388	Chemical shifts as a tool for structure determination. *Methods in Enzymology*, **1994**, 239, 363-92	1.7	744
387	Web-based inference of biological patterns, functions and pathways from metabolomic data using MetaboAnalyst. *Nature Protocols*, **2011**, 6, 743-60	18.8	718
386	Emerging applications of metabolomics in drug discovery and precision medicine. *Nature Reviews Drug Discovery*, **2016**, 15, 473-84	64.1	694
385	VADAR: a web server for quantitative evaluation of protein structure quality. *Nucleic Acids Research* , **2003**, 31, 3316-9	20.1	602
384	Translational biomarker discovery in clinical metabolomics: an introductory tutorial. *Metabolomics*, **2013**, 9, 280-299	4.7	594
383	Circular genome visualization and exploration using CGView. *Bioinformatics*, **2005**, 21, 537-9	7.2	590
382	Escherichia coli K-12: a cooperatively developed annotation snapshot--2005. *Nucleic Acids Research*, **2006**, 34, 1-9	20.1	525
381	The future of NMR-based metabolomics. *Current Opinion in Biotechnology*, **2017**, 43, 34-40	11.4	500
380	Metabolomics: applications to food science and nutrition research. *Trends in Food Science and Technology*, **2008**, 19, 482-493	15.3	476
379	SuperPose: a simple server for sophisticated structural superposition. *Nucleic Acids Research*, **2004**, 32, W590-4	20.1	471
378	Rapid and accurate calculation of protein 1H, 13C and 15N chemical shifts. *Journal of Biomolecular NMR*, **2003**, 26, 215-40	3	452
377	SHIFTX2: significantly improved protein chemical shift prediction. *Journal of Biomolecular NMR*, **2011**, 50, 43-57	3	449
376	MetPA: a web-based metabolomics tool for pathway analysis and visualization. *Bioinformatics*, **2010** , 26, 2342-4	7.2	447

375	MSEA: a web-based tool to identify biologically meaningful patterns in quantitative metabolomic data. *Nucleic Acids Research*, **2010**, 38, W71-7	20.1	412
374	Mass-spectrometry-based metabolomics: limitations and recommendations for future progress with particular focus on nutrition research. *Metabolomics*, **2009**, 5, 435-458	4.7	412
373	Quantitative metabolomics using NMR. *TrAC - Trends in Analytical Chemistry*, **2008**, 27, 228-237	14.6	411
372	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	5	402
371	RefDB: a database of uniformly referenced protein chemical shifts. *Journal of Biomolecular NMR*, **2003**, 25, 173-95	3	357
370	Applications of Machine Learning in Cancer Prediction and Prognosis. *Cancer Informatics*, **2006**, 2, 117693510600200	2.4	352
369	The food metabolome: a window over dietary exposure. *American Journal of Clinical Nutrition*, **2014** , 99, 1286-308	7	335
368	NMR Spectroscopy for Metabolomics Research. *Metabolites*, **2019**, 9,	5.6	330
367	ClassyFire: automated chemical classification with a comprehensive, computable taxonomy. *Journal of Cheminformatics*, **2016**, 8, 61	8.6	327
366	Metabolomics enables precision medicine: "A White Paper, Community Perspective". *Metabolomics*, **2016**, 12, 149	4.7	327
365	A simple method to predict protein flexibility using secondary chemical shifts. *Journal of the American Chemical Society*, **2005**, 127, 14970-1	16.4	325
364	Use of chemical shifts in macromolecular structure determination. *Methods in Enzymology*, **2001**, 338, 3-34	1.7	296
363	CFM-ID: a web server for annotation, spectrum prediction and metabolite identification from tandem mass spectra. *Nucleic Acids Research*, **2014**, 42, W94-9	20.1	278
362	METAGENassist: a comprehensive web server for comparative metagenomics. *Nucleic Acids Research*, **2012**, 40, W88-95	20.1	267
361	The human cerebrospinal fluid metabolome. *Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences*, **2008**, 871, 164-73	3.2	256
360	BASys: a web server for automated bacterial genome annotation. *Nucleic Acids Research*, **2005**, 33, W455-9	20.1	254
359	Competitive fragmentation modeling of ESI-MS/MS spectra for putative metabolite identification. *Metabolomics*, **2015**, 11, 98-110	4.7	237
358	Systems Biology and Multi-Omics Integration: Viewpoints from the Metabolomics Research Community. *Metabolites*, **2019**, 9,	5.6	236

357	SMPDB 2.0: big improvements to the Small Molecule Pathway Database. *Nucleic Acids Research*, **2014**, 42, D478-84	20.1	216
356	SMPDB: The Small Molecule Pathway Database. *Nucleic Acids Research*, **2010**, 38, D480-7	20.1	213
355	Applications of machine learning in cancer prediction and prognosis. *Cancer Informatics*, **2007**, 2, 59-77	2.4	212
354	Advances in metabolite identification. *Bioanalysis*, **2011**, 3, 1769-82	2.1	208
353	The blood exposome and its role in discovering causes of disease. *Environmental Health Perspectives*, **2014**, 122, 769-74	8.4	203
352	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, 16398-403	11.5	198
351	Metabolomics for Investigating Physiological and Pathophysiological Processes. *Physiological Reviews*, **2019**, 99, 1819-1875	47.9	196
350	PolySearch: a web-based text mining system for extracting relationships between human diseases, genes, mutations, drugs and metabolites. *Nucleic Acids Research*, **2008**, 36, W399-405	20.1	180
349	An NMR approach to structural proteomics. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 1825-30	11.5	180
348	CS23D: a web server for rapid protein structure generation using NMR chemical shifts and sequence data. *Nucleic Acids Research*, **2008**, 36, W496-502	20.1	177
347	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	4.7	171
346	Interpreting protein chemical shift data. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2011**, 58, 62-87	10.4	171
345	Protein chemical shift analysis: a practical guide. *Biochemistry and Cell Biology*, **1998**, 76, 153-163	3.6	168
344	T3DB: the toxic exposome database. *Nucleic Acids Research*, **2015**, 43, D928-34	20.1	162
343	pE-DB: a database of structural ensembles of intrinsically disordered and of unfolded proteins. *Nucleic Acids Research*, **2014**, 42, D326-35	20.1	159
342	Current progress in computational metabolomics. *Briefings in Bioinformatics*, **2007**, 8, 279-93	13.4	159
341	Modulation of structure and antibacterial and hemolytic activity by ring size in cyclic gramicidin S analogs. *Journal of Biological Chemistry*, **1996**, 271, 25261-8	5.4	159
340	PREDITOR: a web server for predicting protein torsion angle restraints. *Nucleic Acids Research*, **2006**, 34, W63-9	20.1	158

339	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, D293-5	20.1	156
338	Databases on food phytochemicals and their health-promoting effects. *Journal of Agricultural and Food Chemistry*, **2011**, 59, 4331-48	5.7	151
337	MetaboMiner--semi-automated identification of metabolites from 2D NMR spectra of complex biofluids. *BMC Bioinformatics*, **2008**, 9, 507	3.6	150
336	Accurate, fully-automated NMR spectral profiling for metabolomics. *PLoS ONE*, **2015**, 10, e0124219	3.7	149
335	YMDB: the Yeast Metabolome Database. *Nucleic Acids Research*, **2012**, 40, D815-20	20.1	147
334	MyCompoundID: using an evidence-based metabolome library for metabolite identification. *Analytical Chemistry*, **2013**, 85, 3401-8	7.8	143
333	The human saliva metabolome. *Metabolomics*, **2015**, 11, 1864-1883	4.7	142
332	Applications of metabolomics in drug discovery and development. *Drugs in R and D*, **2008**, 9, 307-22	3.4	142
331	BioTransformer: a comprehensive computational tool for small molecule metabolism prediction and metabolite identification. *Journal of Cheminformatics*, **2019**, 11, 2	8.6	142
330	Livestock metabolomics and the livestock metabolome: A systematic review. *PLoS ONE*, **2017**, 12, e0177675	3.7	140
329	Metabolomics: the principles and potential applications to transplantation. *American Journal of Transplantation*, **2005**, 5, 2814-20	8.7	139
328	Predictive models for breast cancer susceptibility from multiple single nucleotide polymorphisms. *Clinical Cancer Research*, **2004**, 10, 2725-37	12.9	131
327	Gramicidin S is active against both gram-positive and gram-negative bacteria. *International Journal of Peptide and Protein Research*, **1996**, 47, 460-6		130
326	CFM-ID 3.0: Significantly Improved ESI-MS/MS Prediction and Compound Identification. *Metabolites*, **2019**, 9,	5.6	126
325	Metabolomics reveals unhealthy alterations in rumen metabolism with increased proportion of cereal grain in the diet of dairy cows. *Metabolomics*, **2010**, 6, 583-594	4.7	125
324	Metabolomic data processing, analysis, and interpretation using MetaboAnalyst. *Current Protocols in Bioinformatics*, **2011**, Chapter 14, Unit 14.10	24.2	124
323	Improved Glucose Homeostasis in Obese Mice Treated With Resveratrol Is Associated With Alterations in the Gut Microbiome. *Diabetes*, **2017**, 66, 418-425	0.9	121
322	INMEX--a web-based tool for integrative meta-analysis of expression data. *Nucleic Acids Research*, **2013**, 41, W63-70	20.1	119

321	Recommendations of the wwPDB NMR Validation Task Force. *Structure*, **2013**, 21, 1563-70	5.2	117
320	Computational systems biology in drug discovery and development: methods and applications. *Drug Discovery Today*, **2007**, 12, 295-303	8.8	112
319	A review on human fecal metabolomics: Methods, applications and the human fecal metabolome database. *Analytica Chimica Acta*, **2018**, 1030, 1-24	6.6	111
318	Comparison of SDS- and methanol-assisted protein solubilization and digestion methods for Escherichia coli membrane proteome analysis by 2-D LC-MS/MS. *Proteomics*, **2007**, 7, 484-493	4.8	107
317	Nutrimetabolomics: An Integrative Action for Metabolomic Analyses in Human Nutritional Studies. *Molecular Nutrition and Food Research*, **2019**, 63, e1800384	5.9	107
316	Metabolomic fingerprint of heart failure with preserved ejection fraction. *PLoS ONE*, **2015**, 10, e0124844	3.7	106
315	Towards automatic metabolomic profiling of high-resolution one-dimensional proton NMR spectra. *Journal of Biomolecular NMR*, **2011**, 49, 307-23	3	105
314	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	5	105
313	Unusual beta-sheet periodicity in small cyclic peptides. *Nature Structural Biology*, **1998**, 5, 284-8		104
312	CSI 3.0: a web server for identifying secondary and super-secondary structure in proteins using NMR chemical shifts. *Nucleic Acids Research*, **2015**, 43, W370-7	20.1	100
311	Multi-platform characterization of the human cerebrospinal fluid metabolome: a comprehensive and quantitative update. *Genome Medicine*, **2012**, 4, 38	14.4	100
310	ECMDB: the E. coli Metabolome Database. *Nucleic Acids Research*, **2013**, 41, D625-30	20.1	95
309	Recommendations and Standardization of Biomarker Quantification Using NMR-Based Metabolomics with Particular Focus on Urinary Analysis. *Journal of Proteome Research*, **2016**, 15, 360-73	5.6	94
308	T3DB: a comprehensively annotated database of common toxins and their targets. *Nucleic Acids Research*, **2010**, 38, D781-6	20.1	94
307	Improving the accuracy of protein secondary structure prediction using structural alignment. *BMC Bioinformatics*, **2006**, 7, 301	3.6	94
306	Fatty acid composition of developing sea buckthorn (Hippophae rhamnoides L.) berry and the transcriptome of the mature seed. *PLoS ONE*, **2012**, 7, e34099	3.7	93
305	PolySearch2: a significantly improved text-mining system for discovering associations between human diseases, genes, drugs, metabolites, toxins and more. *Nucleic Acids Research*, **2015**, 43, W535-42	20.1	92
304	Identification of bacteria using tandem mass spectrometry combined with a proteome database and statistical scoring. *Analytical Chemistry*, **2004**, 76, 2355-66	7.8	90

303	Computational strategies for metabolite identification in metabolomics. *Bioanalysis*, **2009**, 1, 1579-96	2.1	89
302	Probing the structural determinants of type IIRbeta-turn formation in peptides and proteins. *Journal of the American Chemical Society*, **2002**, 124, 1203-13	16.4	88
301	Synthesis and evaluation of keto-glutamine analogues as potent inhibitors of severe acute respiratory syndrome 3CLpro. *Journal of Medicinal Chemistry*, **2004**, 47, 6113-6	8.3	87
300	Application of the random coil index to studying protein flexibility. *Journal of Biomolecular NMR*, **2008**, 40, 31-48	3	86
299	Solution structure of carnobacteriocin B2 and implications for structure-activity relationships among type IIa bacteriocins from lactic acid bacteria. *Biochemistry*, **1999**, 38, 15438-47	3.2	86
298	Metabolomics and first-trimester prediction of early-onset preeclampsia. *Journal of Maternal-Fetal and Neonatal Medicine*, **2012**, 25, 1840-7	2	85
297	Cancer Metabolomics and the Human Metabolome Database. *Metabolites*, **2016**, 6,	5.6	84
296	Current and Future Perspectives on the Structural Identification of Small Molecules in Biological Systems. *Metabolites*, **2016**, 6,	5.6	84
295	YMDB 2.0: a significantly expanded version of the yeast metabolome database. *Nucleic Acids Research*, **2017**, 45, D440-D445	20.1	83
294	Automated 1H and 13C chemical shift prediction using the BioMagResBank. *Journal of Biomolecular NMR*, **1997**, 10, 329-36	3	81
293	Proteome Analyst: custom predictions with explanations in a web-based tool for high-throughput proteome annotations. *Nucleic Acids Research*, **2004**, 32, W365-71	20.1	80
292	Detailed biophysical characterization of the acid-induced PrP(c) to PrP(I)conversion process. *Biochemistry*, **2011**, 50, 1162-73	3.2	79
291	Exposome-Explorer: a manually-curated database on biomarkers of exposure to dietary and environmental factors. *Nucleic Acids Research*, **2017**, 45, D979-D984	20.1	77
290	Computational Prediction of Electron Ionization Mass Spectra to Assist in GC/MS Compound Identification. *Analytical Chemistry*, **2016**, 88, 7689-97	7.8	76
289	The Bovine Ruminal Fluid Metabolome. *Metabolomics*, **2013**, 9, 360-378	4.7	75
288	Is Cancer a Genetic Disease or a Metabolic Disease?. *EBioMedicine*, **2015**, 2, 478-9	8.8	73
287	ECMDB 2.0: A richer resource for understanding the biochemistry of E. coli. *Nucleic Acids Research*, **2016**, 44, D495-501	20.1	73
286	PROSESS: a protein structure evaluation suite and server. *Nucleic Acids Research*, **2010**, 38, W633-40	20.1	72

285	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, 319-28	3.4	72
284	PHAST, PHASTER and PHASTEST: Tools for finding prophage in bacterial genomes. *Briefings in Bioinformatics*, **2019**, 20, 1560-1567	13.4	71
283	Chemical Composition of Commercial Cow's Milk. *Journal of Agricultural and Food Chemistry*, **2019**, 67, 4897-4914	5.7	70
282	Recommended strategies for spectral processing and post-processing of 1D H-NMR data of biofluids with a particular focus on urine. *Metabolomics*, **2018**, 14, 31	4.7	70
281	Minimum information about a bioactive entity (MIABE). *Nature Reviews Drug Discovery*, **2011**, 10, 661-9	64.1	69
280	Informatics and Data Analytics to Support Exposome-Based Discovery for Public Health. *Annual Review of Public Health*, **2017**, 38, 279-294	20.6	68
279	NMR metabolomics: A look ahead. *Journal of Magnetic Resonance*, **2019**, 306, 155-161	3	68
278	Improving early drug discovery through ADME modelling: an overview. *Drugs in R and D*, **2007**, 8, 349-62	3.4	67
277	The metabolomic profile of umbilical cord blood in neonatal hypoxic ischaemic encephalopathy. *PLoS ONE*, **2012**, 7, e50520	3.7	66
276	NMR: prediction of protein flexibility. *Nature Protocols*, **2006**, 1, 683-8	18.8	65
275	HMDB 5.0: the Human Metabolome Database for 2022.. *Nucleic Acids Research*, **2022**, 50, D622-D631	20.1	65
274	Dynamic relationships among type IIa bacteriocins: temperature effects on antimicrobial activity and on structure of the C-terminal amphipathic alpha helix as a receptor-binding region. *Biochemistry*, **2004**, 43, 9009-20	3.2	64
273	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	2.9	62
272	Small molecule inhibitors of ERCC1-XPF protein-protein interaction synergize alkylating agents in cancer cells. *Molecular Pharmacology*, **2013**, 84, 12-24	4.3	61
271	Identification of novel and known oocyte-specific genes using complementary DNA subtraction and microarray analysis in three different species. *Biology of Reproduction*, **2005**, 73, 63-71	3.9	60
270	CEU Mass Mediator 3.0: A Metabolite Annotation Tool. *Journal of Proteome Research*, **2019**, 18, 797-802	5.6	59
269	Computational approaches to metabolomics. *Methods in Molecular Biology*, **2010**, 593, 283-313	1.4	57
268	PlasMapper: a web server for drawing and auto-annotating plasmid maps. *Nucleic Acids Research*, **2004**, 32, W660-4	20.1	56

267	Microbiome and metabolome modifying effects of several cardiovascular disease interventions in apo-E mice. *Microbiome*, **2017**, 5, 30	16.6	55
266	First-trimester metabolomic detection of late-onset preeclampsia. *American Journal of Obstetrics and Gynecology*, **2013**, 208, 58.e1-7	6.4	55
265	The RCI server: rapid and accurate calculation of protein flexibility using chemical shifts. *Nucleic Acids Research*, **2007**, 35, W531-7	20.1	55
264	Application of solid phase peptide synthesis to engineering PEO–peptide block copolymers for drug delivery. *Colloids and Surfaces B: Biointerfaces*, **2003**, 30, 323-334	6	54
263	Resolution-by-proxy: a simple measure for assessing and comparing the overall quality of NMR protein structures. *Journal of Biomolecular NMR*, **2012**, 53, 167-80	3	52
262	MetATT: a web-based metabolomics tool for analyzing time-series and two-factor datasets. *Bioinformatics*, **2011**, 27, 2455-6	7.2	52
261	Pasture Feeding Changes the Bovine Rumen and Milk Metabolome. *Metabolites*, **2018**, 8,	5.6	51
260	Analogues of bacteriocins: antimicrobial specificity and interactions of leucocin A with its enantiomer, carnobacteriocin B2, and truncated derivatives. *Journal of Medicinal Chemistry*, **2000**, 43, 4579-81	8.3	51
259	Hair metabolomics: identification of fetal compromise provides proof of concept for biomarker discovery. *Theranostics*, **2014**, 4, 953-9	12.1	50
258	A scheme for a flexible classification of dietary and health biomarkers. *Genes and Nutrition*, **2017**, 12, 34	4.3	49
257	PROTEUS2: a web server for comprehensive protein structure prediction and structure-based annotation. *Nucleic Acids Research*, **2008**, 36, W202-9	20.1	49
256	Vl-linker-Vh orientation-dependent expression of single chain Fv-containing an engineered disulfide-stabilized bond in the framework regions. *Journal of Biochemistry*, **1995**, 118, 825-31	3.1	49
255	Metabolomics Profiling of Critically Ill Coronavirus Disease 2019 Patients: Identification of Diagnostic and Prognostic Biomarkers **2020**, 2, e0272		49
254	SPLASH, a hashed identifier for mass spectra. *Nature Biotechnology*, **2016**, 34, 1099-1101	44.5	48
253	Virtual screening and biological evaluation of inhibitors targeting the XPA-ERCC1 interaction. *PLoS ONE*, **2012**, 7, e51329	3.7	48
252	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	4.3	47
251	Association thermodynamics and conformational stability of beta-sheet amyloid beta(17-42) oligomers: effects of E22Q (Dutch) mutation and charge neutralization. *Biophysical Journal*, **2010**, 98, 282-96	2.9	46
250	NMR spectroscopy and protein structure determination: applications to drug discovery and development. *Current Pharmaceutical Biotechnology*, **2005**, 6, 105-20	2.6	46

249	DrugBank and its relevance to pharmacogenomics. *Pharmacogenomics*, **2008**, 9, 1155-62	2.6	45
248	Clinical phenotype clustering in cardiovascular risk patients for the identification of responsive metabotypes after red wine polyphenol intake. *Journal of Nutritional Biochemistry*, **2016**, 28, 114-20	6.3	44
247	GeNMR: a web server for rapid NMR-based protein structure determination. *Nucleic Acids Research*, **2009**, 37, W670-7	20.1	44
246	Metabolomics in monitoring kidney transplants. *Current Opinion in Nephrology and Hypertension*, **2006**, 15, 637-42	3.5	44
245	Validation of metabolomic models for prediction of early-onset preeclampsia. *American Journal of Obstetrics and Gynecology*, **2015**, 213, 530.e1-530.e10	6.4	43
244	Development of a novel virtual screening cascade protocol to identify potential trypanothione reductase inhibitors. *Journal of Medicinal Chemistry*, **2009**, 52, 1670-80	8.3	43
243	International Ring Trial of a High Resolution Targeted Metabolomics and Lipidomics Platform for Serum and Plasma Analysis. *Analytical Chemistry*, **2019**, 91, 14407-14416	7.8	42
242	CAMRA: chemical shift based computer aided protein NMR assignments. *Journal of Biomolecular NMR*, **1998**, 12, 395-405	3	42
241	Hydration effects on the HET-s prion and amyloid-beta fibrillous aggregates, studied with three-dimensional molecular theory of solvation. *Biophysical Journal*, **2008**, 95, 4540-8	2.9	42
240	BacMap: an interactive picture atlas of annotated bacterial genomes. *Nucleic Acids Research*, **2005**, 33, D317-20	20.1	42
239	GC-MS Metabolomics Identifies Metabolite Alterations That Precede Subclinical Mastitis in the Blood of Transition Dairy Cows. *Journal of Proteome Research*, **2017**, 16, 433-446	5.6	41
238	The Bovine Metabolome. *Metabolites*, **2020**, 10,	5.6	40
237	CSI 2.0: a significantly improved version of the Chemical Shift Index. *Journal of Biomolecular NMR*, **2014**, 60, 131-46	3	40
236	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	7.6	40
235	Accurate prediction of protein torsion angles using chemical shifts and sequence homology. *Magnetic Resonance in Chemistry*, **2006**, 44 Spec No, S158-67	2.1	40
234	MovieMaker: a web server for rapid rendering of protein motions and interactions. *Nucleic Acids Research*, **2005**, 33, W358-62	20.1	40
233	Automated bacterial genome analysis and annotation. *Current Opinion in Microbiology*, **2006**, 9, 505-10	7.9	40
232	Learning to predict cancer-associated skeletal muscle wasting from 1H-NMR profiles of urinary metabolites. *Metabolomics*, **2011**, 7, 25-34	4.7	38

231	nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. *Analytical Chemistry*, **2018**, 90, 649-656	7.8	37
230	Simulations of Interdigitated Electrode Interactions with Gold Nanoparticles for Impedance-Based Biosensing Applications. *Sensors*, **2015**, 15, 22192-208	3.8	36
229	Metabolome analysis of 20 taxonomically related benzylisoquinoline alkaloid-producing plants. *BMC Plant Biology*, **2015**, 15, 220	5.3	36
228	Metabolomic analysis for first-trimester Down syndrome prediction. *American Journal of Obstetrics and Gynecology*, **2013**, 208, 371.e1-8	6.4	36
227	Perspective: Dietary Biomarkers of Intake and Exposure-Exploration with Omics Approaches. *Advances in Nutrition*, **2020**, 11, 200-215	10	35
226	Development of isotope labeling liquid chromatography mass spectrometry for mouse urine metabolomics: quantitative metabolomic study of transgenic mice related to Alzheimer's disease. *Journal of Proteome Research*, **2014**, 13, 4457-69	5.6	35
225	Development of Ecom 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, 1222-37	6.1	35
224	PathBank: a comprehensive pathway database for model organisms. *Nucleic Acids Research*, **2020**, 48, D470-D478	20.1	35
223	A sensitive, high-throughput LC-MS/MS method for measuring catecholamines in low volume serum. *Analytica Chimica Acta*, **2018**, 1037, 159-167	6.6	34
222	Metabolomic prediction of fetal congenital heart defect in the first trimester. *American Journal of Obstetrics and Gynecology*, **2014**, 211, 240.e1-240.e14	6.4	34
221	3D-RISM-Dock: A New Fragment-Based Drug Design Protocol. *Journal of Chemical Theory and Computation*, **2012**, 8, 3356-72	6.4	34
220	Exploring human metabolites using the human metabolome database. *Current Protocols in Bioinformatics*, **2009**, Chapter 14, Unit14.8	24.2	33
219	Bioinformatics in drug development and assessment. *Drug Metabolism Reviews*, **2005**, 37, 279-310	7	33
218	NMR solution structure of the precursor for carnobacteriocin B2, an antimicrobial peptide from Carnobacterium piscicola. *FEBS Journal*, **2004**, 271, 1748-56		33
217	Unraveling the unknown areas of the human metabolome: the role of infrared ion spectroscopy. *Journal of Inherited Metabolic Disease*, **2018**, 41, 367-377	5.4	32
216	Metabolomics: a complementary tool in renal transplantation. *Contributions To Nephrology*, **2008**, 160, 76-87	1.6	32
215	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, 1675-84	6.9	31
214	CypReact: A Software Tool for in Silico Reactant Prediction for Human Cytochrome P450 Enzymes. *Journal of Chemical Information and Modeling*, **2018**, 58, 1282-1291	6.1	31

213	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	7	31
212	Characterization of biopharmaceuticals by NMR spectroscopy. *TrAC - Trends in Analytical Chemistry*, **2013**, 48, 96-111	14.6	30
211	A probabilistic approach for validating protein NMR chemical shift assignments. *Journal of Biomolecular NMR*, **2010**, 47, 85-99	3	30
210	A simple method to adjust inconsistently referenced 13C and 15N chemical shift assignments of proteins. *Journal of Biomolecular NMR*, **2005**, 31, 143-8	3	30
209	Developing trends in aptamer-based biosensor devices and their applications. *IEEE Transactions on Biomedical Circuits and Systems*, **2014**, 8, 4-14	5.1	29
208	A simple method to quantitatively measure polypeptide JHNH alpha coupling constants from TOCSY or NOESY spectra. *Journal of Biomolecular NMR*, **1997**, 10, 373-82	3	28
207	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, 181-91	4	27
206	Discovery of small molecule inhibitors that interact with □tubulin. *Chemical Biology and Drug Design*, **2012**, 79, 639-52	2.9	27
205	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. *Nature Structural and Molecular Biology*, **2015**, 22, 433-4	17.6	26
204	Shaking alone induces de novo conversion of recombinant prion proteins to □sheet rich oligomers and fibrils. *PLoS ONE*, **2014**, 9, e98753	3.7	26
203	SEQSEE: a comprehensive program suite for protein sequence analysis. *Bioinformatics*, **1994**, 10, 121-32	7.2	26
202	Functionalized gold nanoparticle-enhanced competitive assay for sensitive small-molecule metabolite detection using surface plasmon resonance. *Analyst, The*, **2017**, 143, 289-296	5	26
201	Metabotyping reveals distinct metabolic alterations in ketotic cows and identifies early predictive serum biomarkers for the risk of disease. *Metabolomics*, **2017**, 13, 1	4.7	25
200	PAMDB: a comprehensive Pseudomonas aeruginosa metabolome database. *Nucleic Acids Research*, **2018**, 46, D575-D580	20.1	25
199	The prion protein binds thiamine. *FEBS Journal*, **2011**, 278, 4002-14	5.7	25
198	Identification of a novel archaebacterial thioredoxin: determination of function through structure. *Biochemistry*, **2002**, 41, 4760-70	3.2	25
197	Computational systems biology in cancer: modeling methods and applications. *Gene Regulation and Systems Biology*, **2007**, 1, 91-110	2	25
196	A simple method to measure protein side-chain mobility using NMR chemical shifts. *Journal of the American Chemical Society*, **2013**, 135, 14536-9	16.4	24

195	Lipopolysaccharide induced conversion of recombinant prion protein. *Prion*, **2014**, 8,	2.3	24
194	Chapter 3: Small molecules and disease. *PLoS Computational Biology*, **2012**, 8, e1002805	5	24
193	Genomic sequence and activity of KS10, a transposable phage of the Burkholderia cepacia complex. *BMC Genomics*, **2008**, 9, 615	4.5	24
192	Dynamic cellular automata: an alternative approach to cellular simulation. *In Silico Biology*, **2005**, 5, 139-61	2.1	24
191	Urinary Metabolomics for Noninvasive Detection of Antibody-Mediated Rejection in Children After Kidney Transplantation. *Transplantation*, **2017**, 101, 2553-2561	1.8	23
190	Salmonella phages and prophages: genomics, taxonomy, and applied aspects. *Methods in Molecular Biology*, **2015**, 1225, 237-87	1.4	23
189	In silico identification of genes in bacteriophage DNA. *Methods in Molecular Biology*, **2009**, 502, 57-89	1.4	23
188	NMR solution structures of the apo and peptide-inhibited human rhinovirus 3C protease (Serotype 14): structural and dynamic comparison. *Biochemistry*, **2007**, 46, 12945-58	3.2	22
187	Magnetic Resonance Diagnostics: A New Technology for High-Throughput Clinical Diagnostics. *Clinical Chemistry*, **2001**, 47, 1918-1921	5.5	22
186	Using DrugBank for In Silico Drug Exploration and Discovery. *Current Protocols in Bioinformatics*, **2016**, 54, 14.4.1-14.4.31	24.2	22
185	Development and Validation of a High-Throughput Mass Spectrometry Based Urine Metabolomic Test for the Detection of Colonic Adenomatous Polyps. *Metabolites*, **2017**, 7,	5.6	21
184	Molecular signatures of end-stage heart failure. *Journal of Cardiac Failure*, **2011**, 17, 867-74	3.3	21
183	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, 7536-45	3.2	21
182	Comparative analysis of essential collective dynamics and NMR-derived flexibility profiles in evolutionarily diverse prion proteins. *Prion*, **2011**, 5, 188-200	2.3	21
181	PepTool and GeneTool: platform-independent tools for biological sequence analysis. *Methods in Molecular Biology*, **2000**, 132, 93-113	1.4	21
180	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		21
179	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	6.1	20
178	Transformation of polyphenols found in pigmented gluten-free flours during in vitro large intestinal fermentation. *Food Chemistry*, **2019**, 298, 125068	8.5	20

177	A High-Performing Plasma Metabolite Panel for Early-Stage Lung Cancer Detection. *Cancers*, **2020**, 12,	6.6	20
176	Metabolomic determination of pathogenesis of late-onset preeclampsia. *Journal of Maternal-Fetal and Neonatal Medicine*, **2017**, 30, 658-664	2	20
175	Pathways with PathWhiz. *Nucleic Acids Research*, **2015**, 43, W552-9	20.1	20
174	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, 317-28	6.1	20
173	Prediction of skeletal muscle and fat mass in patients with advanced cancer using a metabolomic approach. *Journal of Nutrition*, **2012**, 142, 14-21	4.1	20
172	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		20
171	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	2	20
170	Metabolomics Approach Reveals Altered Plasma Amino Acid and Sphingolipid Profiles Associated with Patholological State in Transition Dairy Cows. *Current Metabolomics*, **2015**, 2, 184-195	1	19
169	PA-GOSUB: a searchable database of model organism protein sequences with their predicted Gene Ontology molecular function and subcellular localization. *Nucleic Acids Research*, **2005**, 33, D147-53	20.1	19
168	Assessing the performance of genome-wide association studies for predicting disease risk. *PLoS ONE*, **2019**, 14, e0220215	3.7	19
167	FOBI: an ontology to represent food intake data and associate it with metabolomic data. *Database: the Journal of Biological Databases and Curation*, **2020**, 2020,	5	18
166	Sildenafil Therapy Normalizes the Aberrant Metabolomic Profile in the Comt(-/-) Mouse Model of Preeclampsia/Fetal Growth Restriction. *Scientific Reports*, **2015**, 5, 18241	4.9	18
165	Using multiple structural proteomics approaches for the characterization of prion proteins. *Journal of Proteomics*, **2013**, 81, 31-42	3.9	17
164	Unraveling the meaning of chemical shifts in protein NMR. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2017**, 1865, 1564-1576	4	17
163	Resolution-enhanced native acidic gel electrophoresis: a method for resolving, sizing, and quantifying prion protein oligomers. *Analytical Biochemistry*, **2012**, 426, 54-62	3.1	17
162	GelScape: a web-based server for interactively annotating, manipulating, comparing and archiving 1D and 2D gel images. *Bioinformatics*, **2004**, 20, 976-8	7.2	17
161	Serum metabolomic markers for traumatic brain injury: a mouse model. *Metabolomics*, **2016**, 12, 1	4.7	17
160	Detecting Renal Allograft Inflammation Using Quantitative Urine Metabolomics and CXCL10. *Transplantation Direct*, **2016**, 2, e78	2.3	16

159	Metabolomic profiling of the excretory-secretory products of hookworm and whipworm. *Metabolomics*, **2019**, 15, 101	4.7	16
158	Metabolomic analysis for first-trimester trisomy 18 detection. *American Journal of Obstetrics and Gynecology*, **2013**, 209, 65.e1-9	6.4	16
157	PPT-DB: the protein property prediction and testing database. *Nucleic Acids Research*, **2008**, 36, D222-9	20.1	16
156	Dietary and metabolomic determinants of relapse in ulcerative colitis patients: A pilot prospective cohort study. *World Journal of Gastroenterology*, **2017**, 23, 3890-3899	5.6	16
155	MarkerDB: an online database of molecular biomarkers. *Nucleic Acids Research*, **2021**, 49, D1259-D1267	20.1	16
154	Comprehensive Targeted Metabolomic Assay for Urine Analysis. *Analytical Chemistry*, **2020**, 92, 10627-10634	7.8	15
153	Nano-Optomechanical Systems for Gas Chromatography. *Nano Letters*, **2016**, 16, 6975-6981	11.5	15
152	The use of metabolomics in population-based research. *Advances in Nutrition*, **2014**, 5, 785-8	10	15
151	Progeny of tobacco mosaic virus-infected Nicotiana tabacum plants exhibit trans-generational changes in metabolic profiles. *Biocatalysis and Agricultural Biotechnology*, **2012**, 1, 115-123	4.2	15
150	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	5.7	15
149	3D-RISM-KH approach for biomolecular modelling at nanoscale: thermodynamics of fibril formation and beyond. *Molecular Simulation*, **2011**, 37, 718-728	2	15
148	Exposome-Explorer 2.0: an update incorporating candidate dietary biomarkers and dietary associations with cancer risk. *Nucleic Acids Research*, **2020**, 48, D908-D912	20.1	15
147	Metabolomic prediction of endometrial cancer. *Metabolomics*, **2017**, 14, 6	4.7	15
146	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	4.3	13
145	Identification of candidate biomarkers of brain damage in a mouse model of closed head injury: a metabolomic pilot study. *Metabolomics*, **2016**, 12, 1	4.7	13
144	Brassica villosa, a system for studying non-glandular trichomes and genes in the Brassicas. *Plant Molecular Biology*, **2014**, 85, 519-39	4.6	13
143	Defects in fatty acid amide hydrolase 2 in a male with neurologic and psychiatric symptoms. *Orphanet Journal of Rare Diseases*, **2015**, 10, 38	4.2	13
142	Exploring the essential collective dynamics of interacting proteins: application to prion protein dimers. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 1847-65	4.2	13

141	BacMap: an up-to-date electronic atlas of annotated bacterial genomes. *Nucleic Acids Research*, **2012**, 40, D599-604	20.1	13
140	Complete 1H and non-carbonylic 13C assignments of native hen egg-white lysozyme. *Journal of Biomolecular NMR*, **2000**, 17, 83-4	3	13
139	Nanopore analysis of wild-type and mutant prion protein (PrP(C)): single molecule discrimination and PrP(C) kinetics. *PLoS ONE*, **2013**, 8, e54982	3.7	13
138	Targeted Metabolic Profiling of Post-Mortem Brain from Infants Who Died from Sudden Infant Death Syndrome. *Journal of Proteome Research*, **2017**, 16, 2587-2596	5.6	12
137	Recombinant Incretin-Secreting Microbe Improves Metabolic Dysfunction in High-Fat Diet Fed Rodents. *Scientific Reports*, **2017**, 7, 13523	4.9	12
136	An improved method to detect correct protein folds using partial clustering. *BMC Bioinformatics*, **2013**, 14, 11	3.6	12
135	Differential metabolite profiles and salinity tolerance between two genetically related brown-seeded and yellow-seeded Brassica carinata lines. *Plant Science*, **2013**, 198, 17-26	5.3	12
134	Metabolomic analysis of cold acclimation of Arctic Mesorhizobium sp. strain N33. *PLoS ONE*, **2013**, 8, e84801	3.7	12
133	ORB, a homology-based program for the prediction of protein NMR chemical shifts. *Journal of Biomolecular NMR*, **1997**, 10, 165-179	3	12
132	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	6.6	12
131	Peptide rescue of an N-terminal truncation of the Stoffel fragment of taq DNA polymerase. *Protein Science*, **1996**, 5, 1785-92	6.3	12
130	BioSpider: a web server for automating metabolome annotations. *Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing*, **2007**, 145-56	1.3	12
129	Use of a liposome antigen delivery system to alter immune responses in vivo. *Journal of Pharmaceutical Sciences*, **1998**, 87, 1428-32	3.9	11
128	PSA fluoroimmunoassays using anti-PSA ScFv and quantum-dot conjugates. *Nanomedicine*, **2008**, 3, 475-83	5.6	11
127	Structural and functional characterization of a thioredoxin-like protein (Mt0807) from Methanobacterium thermoautotrophicum. *Biochemistry*, **2003**, 42, 8001-10	3.2	11
126	The BioTools Suite. A comprehensive suite of platform-independent bioinformatics tools. *Molecular Biotechnology*, **2001**, 19, 59-77	3	11
125	Targeted metabolomics identifies high performing diagnostic and prognostic biomarkers for COVID-19. *Scientific Reports*, **2021**, 11, 14732	4.9	11
124	A simple in vitro assay for assessing the efficacy, mechanisms and kinetics of anti-prion fibril compounds. *Prion*, **2018**, 12, 280-300	2.3	11

123	CFM-ID 4.0: More Accurate ESI-MS/MS Spectral Prediction and Compound Identification. *Analytical Chemistry*, **2021**, 93, 11692-11700	7.8	11
122	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	1.8	10
121	Introduction to Cheminformatics. *Current Protocols in Bioinformatics*, **2016**, 53, 14.1.1-14.1.21	24.2	10
120	Non-invasive staging of chronic kidney allograft damage using urine metabolomic profiling. *Pediatric Transplantation*, **2018**, 22, e13226	1.8	10
119	Molecular docking of thiamine reveals similarity in binding properties between the prion protein and other thiamine-binding proteins. *Journal of Molecular Modeling*, **2013**, 19, 5225-35	2	10
118	Introduction to cheminformatics. *Current Protocols in Bioinformatics*, **2007**, Chapter 14, Unit 14.1	24.2	10
117	Computational Systems Biology in Cancer: Modeling Methods and Applications. *Gene Regulation and Systems Biology*, **2007**, 1, 117762500700100	2	10
116	Production of an anti-prostate-specific antigen single-chain antibody fragment from Pichia pastoris. *Protein Expression and Purification*, **2001**, 23, 419-25	2	10
115	Constrained multiple sequence alignment using XALIGN. *Bioinformatics*, **1994**, 10, 687-8	7.2	10
114	Bioinformatics in Drug Development and Assessment. *Drug Metabolism Reviews*, **2005**, 37, 279-310	7	10
113	In silico studies and fluorescence binding assays of potential anti-prion compounds reveal an important binding site for prion inhibition from PrP(C) to PrP(Sc). *European Journal of Medicinal Chemistry*, **2015**, 91, 118-31	6.8	9
112	The role of the Human Metabolome Database in inborn errors of metabolism. *Journal of Inherited Metabolic Disease*, **2018**, 41, 329-336	5.4	9
111	Protein contact order prediction from primary sequences. *BMC Bioinformatics*, **2008**, 9, 255	3.6	9
110	Solution structures of reduced and oxidized bacteriophage T4 glutaredoxin. *Journal of Biomolecular NMR*, **2004**, 29, 85-90	3	9
109	Impact of Bovine Diet on Metabolomic Profile of Skim Milk and Whey Protein Ingredients. *Metabolites*, **2019**, 9,	5.6	9
108	Protocols for NMR Analysis in Livestock Metabolomics. *Methods in Molecular Biology*, **2019**, 1996, 311-324	1.4	8
107	Accessible surface area from NMR chemical shifts. *Journal of Biomolecular NMR*, **2015**, 62, 387-401	3	8
106	The Urinary Metabolome of Healthy Newborns. *Metabolites*, **2020**, 10,	5.6	8

105	Using isotopically-coded hydrogen peroxide as a surface modification reagent for the structural characterization of prion protein aggregates. *Journal of Proteomics*, **2014**, 100, 160-6	3.9	8
104	Experimental and computational study of the interaction of novel colchicinoids with a recombinant human β/α-tubulin heterodimer. *Chemical Biology and Drug Design*, **2013**, 82, 60-70	2.9	8
103	A robust algorithm for optimizing protein structures with NMR chemical shifts. *Journal of Biomolecular NMR*, **2015**, 63, 255-64	3	8
102	Discovering drug targets through the web. *Comparative Biochemistry and Physiology Part D: Genomics and Proteomics*, **2007**, 2, 9-17	2	8
101	Metabolomics in Humans and Other Mammals253-288		8
100	Chemical language models enable navigation in sparsely populated chemical space. *Nature Machine Intelligence*, **2021**, 3, 759-770	22.5	8
99	Targeted metabolomics highlights perturbed metabolism in the brain of autism spectrum disorder sufferers. *Metabolomics*, **2020**, 16, 59	4.7	7
98	Initial Structural Models of the Aβ42 Dimer from Replica Exchange Molecular Dynamics Simulations. *ACS Omega*, **2017**, 2, 7621-7636	3.9	7
97	Candidate serum metabolite biomarkers of residual feed intake and carcass merit in sheep. *Journal of Animal Science*, **2020**, 98,	0.7	7
96	Tools for Protein Technologies325-344		7
95	Systems Biology Resources Arising from the Human Metabolome Project **2012**, 157-175		7
94	A fast, sensitive, single-step colorimetric dipstick assay for quantifying ascorbic acid in urine. *Analytical Biochemistry*, **2019**, 580, 1-13	3.1	6
93	Urinary Metabolomics around Parturition Identifies Metabolite Alterations in Dairy Cows Affected Postpartum by Lameness: Preliminary Study. *Dairy*, **2020**, 1, 2	2.6	6
92	The bacterial nanorecorder: engineering E. coli to function as a chemical recording device. *PLoS ONE*, **2011**, 6, e27559	3.7	6
91	Facile measurement of polypeptide JHNH alpha coupling constants from HMQC-J spectra. *Journal of Biomolecular NMR*, **1998**, 11, 329-36	3	6
90	Characterization of a highly potent antimicrobial peptide microcin N from uropathogenic Escherichia coli. *FEMS Microbiology Letters*, **2016**, 363,	2.9	6
89	A Simple and Convenient Synthesis of Unlabeled and C-Labeled 3-(3-Hydroxyphenyl)-3-Hydroxypropionic Acid and Its Quantification in Human Urine Samples. *Metabolites*, **2018**, 8,	5.6	6
88	Identification of serum metabolites associated with the risk of metritis in transition dairy cows. *Canadian Journal of Animal Science*, **2018**, 98, 525-537	0.9	5

87	Isolation of soluble scFv antibody fragments specific for small biomarker molecule, L-Carnitine, using phage display. *Journal of Immunological Methods*, **2016**, 428, 9-19	2.5	5
86	In silico drug exploration and discovery using DrugBank. *Current Protocols in Bioinformatics*, **2007**, Chapter 14, Unit 14.4	24.2	5
85	Design, synthesis and characterization of a water-soluble β-sheet peptide. *Techniques in Protein Chemistry*, **1995**, 6, 451-457		5
84	Mass-spec-based urinary metabotyping around parturition identifies screening biomarkers for subclinical mastitis in dairy cows. *Research in Veterinary Science*, **2020**, 129, 39-52	2.5	5
83	Serum Metabolite Biomarkers for Predicting Residual Feed Intake (RFI) of Young Angus Bulls. *Metabolites*, **2020**, 10,	5.6	5
82	Role of polysaccharide and lipid in lipopolysaccharide induced prion protein conversion. *Prion*, **2016**, 10, 466-483	2.3	5
81	Non-invasive Point-of-Care Device To Diagnose Acute Mesenteric Ischemia. *ACS Sensors*, **2018**, 3, 2296-2302	9.2	5
80	Metabolomic Data Exploration and Analysis with the Human Metabolome Database. *Methods in Molecular Biology*, **2020**, 2104, 165-184	1.4	5
79	Non-invasive differentiation of non-rejection kidney injury from acute rejection in pediatric renal transplant recipients. *Pediatric Transplantation*, **2019**, 23, e13364	1.8	4
78	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	5.7	4
77	An impedance detection circuit for applications in a portable biosensor system **2016**,		4
76	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	4.2	4
75	A simple and sensitive biosensor for rapid detection of nanoparticles in water. *Journal of Nanoparticle Research*, **2014**, 16, 1	2.3	4
74	Online Databases and Web Servers for Drug Metabolism Research. *Methods and Principles in Medicinal Chemistry*, **2014**, 53-74	0.4	4
73	Metallotyping of ketotic dairy cows reveals major alterations preceding, associating, and following the disease occurrence. *Metabolomics*, **2017**, 13, 1	4.7	4
72	Identification and characterization of ?H111-1: A novel myovirus with broad activity against clinical isolates of. *Bacteriophage*, **2013**, 3, e26649		4
71	Solution Structure of MTH0776 from Methanobacterium thermoautotrophicum. *Journal of Biomolecular NMR*, **2005**, 33, 51-6	3	4
70	A deep generative model enables automated structure elucidation of novel psychoactive substances. *Nature Machine Intelligence*, **2021**, 3, 973-984	22.5	4

69	Automated Tools for the Analysis of 1D-NMR and 2D-NMR Spectra. *Methods in Molecular Biology*, **2019**, 2037, 429-449	1.4	4
68	A Comprehensive Targeted Metabolomics Assay for Crop Plant Sample Analysis. *Metabolites*, **2021**, 11,	5.6	4
67	CyProduct: A Software Tool for Accurately Predicting the Byproducts of Human Cytochrome P450 Metabolism. *Journal of Chemical Information and Modeling*, **2021**, 61, 3128-3140	6.1	4
66	First-trimester metabolomic prediction of stillbirth. *Journal of Maternal-Fetal and Neonatal Medicine*, **2019**, 32, 3435-3441	2	4
65	Predicting PAMPA permeability using the 3D-RISM-KH theory: are we there yet?. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 261-269	4.2	4
64	A Multi-Platform Metabolomics Approach Identifies Urinary Metabolite Signatures That Differentiate Ketotic From Healthy Dairy Cows. *Frontiers in Veterinary Science*, **2021**, 8, 595983	3.1	4
63	Peptide-based fluorescence biosensors for detection/measurement of nanoparticles. *Analytical and Bioanalytical Chemistry*, **2017**, 409, 903-915	4.4	3
62	Preparation and characterization of a highly soluble A peptide variant. *Protein Expression and Purification*, **2019**, 164, 105480	2	3
61	Porous Nanophotonic Optomechanical Beams for Enhanced Mass Adsorption. *ACS Sensors*, **2019**, 4, 1197-1202	9.1	3
60	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	2.3	3
59	Effect of Diet on the Vitamin B Profile of Bovine Milk-Based Protein Ingredients. *Foods*, **2020**, 9,	4.9	3
58	A Web Tool for Generating High Quality Machine-readable Biological Pathways. *Journal of Visualized Experiments*, **2017**,	1.6	3
57	Exploring the Human Metabolome by Nuclear Magnetic Resonance Spectroscopy and Mass Spectrometry	3-29	3
56	Evidence for copurification of micronuclei in sucrose density gradient-enriched plasma membranes from cell lines. *Analytical Biochemistry*, **2010**, 396, 69-75	3.1	3
55	Complete 1H, 13C and 15N backbone assignments for the hepatitis A virus 3C protease. *Journal of Biomolecular NMR*, **2001**, 19, 187-8	3	3
54	Emerging technologies and their impact on regulatory science. *Experimental Biology and Medicine*, **2021**, 15353702211052280	3.7	3
53	Identifying putative drug targets and potential drug leads: starting points for virtual screening and docking. *Methods in Molecular Biology*, **2008**, 443, 333-51	1.4	3
52	Gut Microenvironment and Bacterial Invasion in Paediatric Inflammatory Bowel Diseases. *Journal of Pediatric Gastroenterology and Nutrition*, **2020**, 71, 624-632	2.8	3

51	Workshop report: Toward the development of a human whole stool reference material for metabolomic and metagenomic gut microbiome measurements. *Metabolomics*, **2020**, 16, 119	4.7	3
50	Excretory/Secretory Metabolome of the Zoonotic Roundworm Parasite. *Biomolecules*, **2020**, 10,	5.9	3
49	Rapid and reliable protein structure determination via chemical shift threading. *Journal of Biomolecular NMR*, **2018**, 70, 33-51	3	3
48	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 PrP to PrP with lower IC in ScN2a cells. *Bioorganic and Medicinal Chemistry*, **2017**, 25, 5875-5888	3.4	2
47	Serum metabolomics identifies metabolite panels that differentiate lame dairy cows from healthy ones. *Metabolomics*, **2020**, 16, 73	4.7	2
46	Growth of Malignant Non-CNS Tumors Alters Brain Metabolome. *Frontiers in Genetics*, **2018**, 9, 41	4.5	2
45	DrugBank55-65		2
44	Spatiotemporal integration of molecular and anatomical data in virtual reality using semantic mapping. *International Journal of Nanomedicine*, **2009**, 4, 79-89	7.3	2
43	Solid phase synthesis of acylglycine human metabolites. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 6706-8	2.9	2
42	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		2
41	Backbone 1H, 15N and 13C assignments for the human rhinovirus 3C protease (serotype 14). *Journal of Biomolecular NMR*, **2003**, 26, 85-6	3	2
40	An improved synthesis of □13C glycine and heteronuclear NMR studies of its incorporation into thioredoxin. *Journal of Labelled Compounds and Radiopharmaceuticals*, **1992**, 31, 1019-1028	1.9	2
39	Metabolomics in Exercise and Sports: A Systematic Review. *Sports Medicine*, **2021**, 1	10.6	2
38	Serum metabolic fingerprinting of pre-lameness dairy cows by GC-MS reveals typical profiles that can identify susceptible cows. *Journal of Proteomics*, **2020**, 213, 103620	3.9	2
37	Solvent Composition Effects on the Structural Properties of the A□42 Monomer from the 3D-RISM-KH Molecular Theory of Solvation. *Journal of Physical Chemistry B*, **2019**, 123, 2491-2506	3.4	2
36	Food Constituent and Food Metabolite Databases **2021**, 2-18		2
35	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	4	2
34	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	5.6	2

33	Immunometabolic signatures predict risk of progression to sepsis in COVID-19. *PLoS ONE*, **2021**, 16, e0256784	3.7	2
32	A Targeted Serum Metabolomics GC-MS Approach Identifies Predictive Blood Biomarkers for Retained Placenta in Holstein Dairy Cows. *Metabolites*, **2021**, 11,	5.6	2
31	Simulating electrical properties of interdigitated electrode designs for impedance-based biosensing applications **2015**,		1
30	Value-based healthcare delivery through metabolomics-based personalized health platform. *Healthcare Management Forum*, **2020**, 33, 126-134	1.7	1
29	Proteins: Hormones, Enzymes, and Monoclonal Antibodies Background691-736		1
28	Complete 1H, 13C and 15N NMR assignments of MTH0776 from Methanobacterium thermoautotrophicum. *Journal of Biomolecular NMR*, **2004**, 30, 459-60	3	1
27	Blood Metabolomic Phenotyping of Dry Cows Could Predict the High Milk Somatic Cells in Early Lactation Preliminary Results. *Dairy*, **2022**, 3, 59-77	2.6	1
26	Assessing the performance of genome-wide association studies for predicting disease risk		1
25	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	4.5	1
24	Drug-target discovery in silico: using the web to identify novel molecular targets for drug action. *SEB Experimental Biology Series*, **2007**, 58, 145-76		1
23	Advances in Metabolomics-Driven Diagnostic Breeding and Crop Improvement. *Metabolites*, **2022**, 12, 511	5.6	1
22	A Canadian Study of Cisplatin Metabolomics and Nephrotoxicity (ACCENT): A Clinical Research Protocol. *Canadian Journal of Kidney Health and Disease*, **2021**, 8, 20543581211057708	2.3	0
21	Urinary metabolomics to develop predictors for pediatric acute kidney injury.. *Pediatric Nephrology*, **2022**, 1	3.2	0
20	CpG-ODN induced antimicrobial immunity in neonatal chicks involves a substantial shift in serum metabolic profiles. *Scientific Reports*, **2021**, 11, 9028	4.9	0
19	Cloning and high-level expression of monomeric human superoxide dismutase 1 (SOD1) and its interaction with pyrimidine analogs. *PLoS ONE*, **2021**, 16, e0247684	3.7	0
18	Systemic inflammation and metabolic disturbances underlie inpatient mortality among ill children with severe malnutrition.. *Science Advances*, **2022**, 8, eabj6779	14.3	0
17	Urinary Organic Acids Increase After Clinical Stabilization of Hospitalized Children With Severe Acute Malnutrition. *Food and Nutrition Bulletin*, **2019**, 40, 532-543	1.8	
16	Shouldn 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	64.1	

15	Protein Contact Order Prediction: Update **2013**, 205-216	
14	Bioinformatics for Metabolomics **2009**, 581-599	
13	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, 1060-8	3.2
12	Software Tools for Proteomics Technologies323-352	
11	Metabolomic Fingerprint of Behavioral Changes in Response to Full-Spectrum Cannabis Extracts.. *Frontiers in Pharmacology*, **2022**, 13, 831052	5.6
10	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	2.5
9	On the Use of NMR in Complex Biological Systems: NMR Studies of Calcium Sensitive Interactions amongst Muscle Proteins **1996**, 275-284	
8	Identifying putative drug targets and potential drug leads: starting points for virtual screening and docking. *Methods in Molecular Biology*, **2015**, 1215, 425-44	1.4
7	Proteins: Hormones, Enzymes, and Monoclonal AntibodiesBackground1	
6	Picornain 3C (human rhinovirus) **2013**, 2402-2406	
5	A longitudinal dataset of incidence and intervention policy impacts regarding the COVID-19 pandemic in Canadian provinces. *Data in Brief*, **2021**, 38, 107381	1.2
4	Assessing the performance of genome-wide association studies for predicting disease risk **2019**, 14, e0220215	
3	Assessing the performance of genome-wide association studies for predicting disease risk **2019**, 14, e0220215	
2	Assessing the performance of genome-wide association studies for predicting disease risk **2019**, 14, e0220215	
1	Assessing the performance of genome-wide association studies for predicting disease risk **2019**, 14, e0220215	