Shoba Ranganathan

List of Publications by Year in Descending Order

190 papers	6,118 citations	40 h-index	72 g-index
223 ext. papers	6,820 ext. citations	6.7 avg, IF	5.49 L-index

#	Paper	IF	Citations
190	A Bioinformatics Approach to Mine the Microbial Proteomic Profile of COVID-19 Mass Spectrometry Data. *Applied Microbiology*, **2022**, 2, 150-164		1
189	Leveraging homologies for cross-species plasma proteomics in ungulates using data-independent acquisition. *Journal of Proteomics*, **2022**, 250, 104384	3.9	0
188	ML218 HCl Is More Efficient Than Capsaicin in Inhibiting Bacterial Antigen-Induced Cal 27 Oral Cancer Cell Proliferation. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
187	BIO-GATS: A Tool for Automated GPCR Template Selection Through a Biophysical Approach for Homology Modeling. *Frontiers in Molecular Biosciences*, **2021**, 8, 617176	5.6	0
186	Mass spectrometry-based protein identification in proteomics-a review. *Briefings in Bioinformatics*, **2021**, 22, 1620-1638	13.4	18
185	Bacterial Antigens Reduced the Inhibition Effect of Capsaicin on Cal 27 Oral Cancer Cell Proliferation. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	2
184	A two-stage computational approach to predict novel ligands for a chemosensory receptor. *Current Research in Structural Biology*, **2020**, 2, 213-221	2.8	1
183	iSwathX 2.0 for Processing DDA Spectral Libraries for DIA Data Analysis. *Current Protocols in Bioinformatics*, **2020**, 70, e101	24.2	1
182	Enhancing protein backbone angle prediction by using simpler models of deep neural networks. *Scientific Reports*, **2020**, 10, 19430	4.9	6
181	Structural bioinformatics analysis of variants on GPCR function. *Current Opinion in Structural Biology*, **2019**, 55, 161-177	8.1	3
180	Bioinformatics approaches for improving seminal plasma proteome analysis. *Theriogenology*, **2019**, 137, 43-49	2.8	
179	Applications of machine learning in GPCR bioactive ligand discovery. *Current Opinion in Structural Biology*, **2019**, 55, 66-76	8.1	20
178	APBioNet's annual International Conference on Bioinformatics (InCoB) returns to India in 2018. *BMC Genomics*, **2019**, 19, 266	4.5	0
177	Diverse dynamics features of novel protein kinase C (PKC) isozymes determine the selectivity of a fluorinated balanol analogue for PKC. *BMC Bioinformatics*, **2019**, 19, 342	3.6	1
176	iSwathX: an interactive web-based application for extension of DIA peptide reference libraries. *Bioinformatics*, **2019**, 35, 538-539	7.2	11
175	Identification of Proteins From Proteomic Analysis **2019**, 855-870		1
174	Protocol for Protein Structure Modelling **2019**, 252-272		6

#	Title	IF	Cit
173	Structure-Based Drug Design Workflow **2019**, 273-282		2
172	Quantification of Proteins From Proteomic Analysis **2019**, 871-890		1
171	Looking for Missing Proteins **2019**,		1
170	Prediction of novel mouse TLR9 agonists using a random forest approach. *BMC Molecular and Cell Biology*, **2019**, 20, 56	2.7	1
169	Molecular Dynamics Pinpoint the Global Fluorine Effect in Balanoid Binding to PKCand PKA. *Journal of Chemical Information and Modeling*, **2018**, 58, 511-519	6.1	3
168	Computational analysis of the receptor binding specificity of novel influenza A/H7N9 viruses. *BMC Genomics*, **2018**, 19, 88	4.5	7
167	Clinically Relevant Post-Translational Modification Analyses-Maturing Workflows and Bioinformatics Tools. *International Journal of Molecular Sciences*, **2018**, 20,	6.3	23
166	PhoglyStruct: Prediction of phosphoglycerylated lysine residues using structural properties of amino acids. *Scientific Reports*, **2018**, 8, 17923	4.9	24
165	Imaginative Order from Reasonable Chaos: Conformation-Driven Activity and Reactivity in Exploring Proteinligand Interactions. *Australian Journal of Chemistry*, **2018**, 71, 917	1.2	
164	Role of solvent accessibility for aggregation-prone patches in protein folding. *Scientific Reports*, **2018**, 8, 12896	4.9	7
163	Accelerating the search for the missing proteins in the human proteome. *Nature Communications*, **2017**, 8, 14271	17.4	73
162	Divergent response of homologous ATP sites to stereospecific ligand fluorination for selectivity enhancement. *Organic and Biomolecular Chemistry*, **2017**, 15, 1570-1574	3.9	8
161	De Novo Peptide Sequencing: Deep Mining of High-Resolution Mass Spectrometry Data. *Methods in Molecular Biology*, **2017**, 1549, 119-134	1.4	7
160	A Systematic Bioinformatics Approach to Identify High Quality Mass Spectrometry Data and Functionally Annotate Proteins and Proteomes. *Methods in Molecular Biology*, **2017**, 1549, 163-176	1.4	3
159	Exploration of charge states of balanol analogues acting as ATP-competitive inhibitors in kinases. *BMC Bioinformatics*, **2017**, 18, 572	3.6	5
158	Human Prestin: A Candidate PE1 Protein Lacking Stringent Mass Spectrometric Evidence?. *Journal of Proteome Research*, **2017**, 16, 4531-4535	5.6	4
157	Prediction of interface residue based on the features of residue interaction network. *Journal of Theoretical Biology*, **2017**, 432, 49-54	2.3	8
156	Bioinformatics and systems biology research update from the 15 International Conference on Bioinformatics (InCoB2016). *BMC Bioinformatics*, **2016**, 17, 524	3.6	1

155	Systems Proteomics View of the Endogenous Human Claudin Protein Family. *Journal of Proteome Research*, **2016**, 15, 339-59	5.6	17
154	Cracking the nodule worm code advances knowledge of parasite biology and biotechnology to tackle major diseases of livestock. *Biotechnology Advances*, **2015**, 33, 980-91	17.8	18
153	Quest for Missing Proteins: Update 2015 on Chromosome-Centric Human Proteome Project. *Journal of Proteome Research*, **2015**, 14, 3415-31	5.6	50
152	GIW and InCoB are advancing bioinformatics in the Asia-Pacific. *BMC Bioinformatics*, **2015**, 16, I1	3.6	
151	Discrete structural features among interface residue-level classes. *BMC Bioinformatics*, **2015**, 16 Suppl 18, S8	3.6	9
150	Linking structural features of protein complexes and biological function. *Protein Science*, **2015**, 24, 1486-94	3.5	28
149	Coherence analysis discriminates between retroviral integration patterns in CD34(+) cells transduced under differing clinical trial conditions. *Molecular Therapy - Methods and Clinical Development*, **2015**, 2, 15015	6.4	1
148	A novel multiplexed immunoassay identifies CEA, IL-8 and prolactin as prospective markers for DukesⓅstages A-D colorectal cancers. *Clinical Proteomics*, **2015**, 12, 10	5	28
147	Genome of the human hookworm Necator americanus. *Nature Genetics*, **2014**, 46, 261-269	36.3	139
146	A site for direct integrin αvβ3-uPAR interaction from structural modelling and docking. *Journal of Structural Biology*, **2014**, 185, 327-35	3.4	12
145	Protannotator: a semiautomated pipeline for chromosome-wise functional annotation of the "missing" human proteome. *Journal of Proteome Research*, **2014**, 13, 76-83	5.6	13
144	Characterization of the interaction between heterodimeric αvβ6 integrin and urokinase plasminogen activator receptor (uPAR) using functional proteomics. *Journal of Proteome Research*, **2014**, 13, 5956-64	5.6	15
143	InCoB2014: bioinformatics to tackle the data to knowledge challenge. Introduction. *BMC Bioinformatics*, **2014**, 15 Suppl 16, I1	3.6	
142	InCoB2014: Systems Biology update from the Asia-Pacific. Introduction. *BMC Systems Biology*, **2014**, 8 Suppl 4, I1	3.5	1
141	InCoB2014: mining biological data from genomics for transforming industry and health. *BMC Genomics*, **2014**, 15 Suppl 9, I1	4.5	2
140	Transcriptome analysis reveals pathogenicity and evolutionary history of the pathogenic oomycete Pythium insidiosum. *Fungal Biology*, **2014**, 118, 640-53	2.8	22
139	Protein-protein interactions and prediction: a comprehensive overview. *Protein and Peptide Letters*, **2014**, 21, 779-89	1.9	12
138	Structure-based clustering of major histocompatibility complex (MHC) proteins for broad-based T-cell vaccine design. *Methods in Molecular Biology*, **2014**, 1184, 503-11	1.4	0

137	Identification of ovarian cancer associated genes using an integrated approach in a Boolean framework. *BMC Systems Biology*, **2013**, 7, 12	3.5	11
136	Simple re-instantiation of small databases using cloud computing. *BMC Genomics*, **2013**, 14 Suppl 5, S13	4.5	6
135	InCoB2013 introduces Systems Biology as a major conference theme. *BMC Systems Biology*, **2013**, 7 Suppl 3, S1	3.5	2
134	The transcriptome of Echinostoma caproni adults: further characterization of the secretome and identification of new potential drug targets. *Journal of Proteomics*, **2013**, 89, 202-14	3.9	15
133	Functional annotation of the human chromosome 7 "missing" proteins: a bioinformatics approach. *Journal of Proteome Research*, **2013**, 12, 2504-10	5.6	16
132	Unlocking the puzzling biology of the black Périgord truffle Tuber melanosporum. *Journal of Proteome Research*, **2013**, 12, 5349-56	5.6	22
131	Vaccine adjuvant informatics **2013**, 123-130		1
130	Database design **2013**, 47-57		
129	Infectious disease informatics **2013**, 99-110		
128	APBioNet-transforming bioinformatics in the Asia-Pacific region. *PLoS Computational Biology*, **2013**, 9, e1003317	5	2
127	Computational T cell vaccine design **2013**, 59-86		
126	Scientific publications and databases **2013**, 21-46		0
125	Biological Data Integration Using Network Models **2013**, 155-174		2
124	High-Throughput Functional Annotation and Data Mining of Fungal Genomes to Identify Therapeutic Targets **2013**, 559-564		
123	Bioinformatics meets parasitology. *Parasite Immunology*, **2012**, 34, 265-75	2.2	18
122	An ethnobotanical study of medicinal plants used by the Yaegl Aboriginal community in northern New South Wales, Australia. *Journal of Ethnopharmacology*, **2012**, 139, 244-55	5	38
121	Whole-genome sequence of Schistosoma haematobium. *Nature Genetics*, **2012**, 44, 221-5	36.3	325
120	TranSeqAnnotator: large-scale analysis of transcriptomic data. *BMC Bioinformatics*, **2012**, 13 Suppl 17, S24	3.6	4

119	An analysis of the transcriptome of Teladorsagia circumcincta: its biological and biotechnological implications. *BMC Genomics*, **2012**, 13 Suppl 7, S10	4.5	16
118	The transcriptome analysis of Strongyloides stercoralis L3i larvae reveals targets for intervention in a neglected disease. *PLoS Neglected Tropical Diseases*, **2012**, 6, e1513	4.8	24
117	Helminth secretome database (HSD): a collection of helminth excretory/secretory proteins predicted from expressed sequence tags (ESTs). *BMC Genomics*, **2012**, 13 Suppl 7, S8	4.5	29
116	Ecological niche modeling of customary medicinal plant species used by Australian Aborigines to identify species-rich and culturally valuable areas for conservation. *Ecological Modelling*, **2011**, 222, 3437-3443	2	26
115	Deep insights into Dictyocaulus viviparus transcriptomes provides unique prospects for new drug targets and disease intervention. *Biotechnology Advances*, **2011**, 29, 261-71	17.8	27
114	Ascaris suum draft genome. *Nature*, **2011**, 479, 529-33	50.4	217
113	Structural diversity of biologically interesting datasets: a scaffold analysis approach. *Journal of Cheminformatics*, **2011**, 3, 30	8.6	28
112	Towards big data science in the decade ahead from ten years of InCoB and the 1st ISCB-Asia Joint Conference. *BMC Bioinformatics*, **2011**, 12 Suppl 13, S1	3.6	15
111	In silico approach to screen compounds active against parasitic nematodes of major socio-economic importance. *BMC Bioinformatics*, **2011**, 12 Suppl 13, S25	3.6	8
110	In silico secretome analysis approach for next generation sequencing transcriptomic data. *BMC Genomics*, **2011**, 12 Suppl 3, S14	4.5	27
109	A comparative structural bioinformatics analysis of inherited mutations in α-D-Mannosidase across multiple species reveals a genotype-phenotype correlation. *BMC Genomics*, **2011**, 12 Suppl 3, S22	4.5	12
108	Molecular similarity and diversity approaches in chemoinformatics. *Drug Development Research*, **2011**, 72, 74-84	5.1	9
107	MPID-T2: a database for sequence-structure-function analyses of pMHC and TR/pMHC structures. *Bioinformatics*, **2011**, 27, 1192-3	7.2	16
106	Understanding TR binding to pMHC complexes: how does a TR scan many pMHC complexes yet preferentially bind to one. *PLoS ONE*, **2011**, 6, e17194	3.7	8
105	A practical, bioinformatic workflow system for large data sets generated by next-generation sequencing. *Nucleic Acids Research*, **2010**, 38, e171	20.1	60
104	Massively parallel sequencing and analysis of the Necator americanus transcriptome. *PLoS Neglected Tropical Diseases*, **2010**, 4, e684	4.8	66
103	Meeting Report from the Second "Minimum Information for Biological and Biomedical Investigations" (MIBBI) workshop. *Standards in Genomic Sciences*, **2010**, 3, 259-66		26
102	Untangling Biological Networks Using Bioinformatics **2010**, 865-892		

101	In Silico Methods for the Analysis of Metabolites and Drug Molecules **2010**, 361-381		
100	Graphs in Bioinformatics **2010**, 191-219		1
99	InCoB2010 - 9th International Conference on Bioinformatics at Tokyo, Japan, September 26-28, 2010. *BMC Bioinformatics*, **2010**, 11 Suppl 7, S1	3.6	1
98	Network analysis of human protein location. *BMC Bioinformatics*, **2010**, 11 Suppl 7, S9	3.6	10
97	Challenges of the next decade for the Asia Pacific region: 2010 International Conference in Bioinformatics (InCoB 2010). *BMC Genomics*, **2010**, 11 Suppl 4, S1	4.5	9
96	Advancing standards for bioinformatics activities: persistence, reproducibility, disambiguation and Minimum Information About a Bioinformatics investigation (MIABi). *BMC Genomics*, **2010**, 11 Suppl 4, S27	4.5	19
95	First transcriptomic analysis of the economically important parasitic nematode, Trichostrongylus colubriformis, using a next-generation sequencing approach. *Infection, Genetics and Evolution*, **2010**, 10, 1199-207	4.5	50
94	pDOCK: a new technique for rapid and accurate docking of peptide ligands to Major Histocompatibility Complexes. *Immunome Research*, **2010**, 6 Suppl 1, S2		28
93	Bioinformatics for Immunomics **2010**,		2
92	Towards a career in bioinformatics. *BMC Bioinformatics*, **2009**, 10 Suppl 15, S1	3.6	5
91	Physiochemical property space distribution among human metabolites, drugs and toxins. *BMC Bioinformatics*, **2009**, 10 Suppl 15, S10	3.6	43
90	A comprehensive assessment of N-terminal signal peptides prediction methods. *BMC Bioinformatics*, **2009**, 10 Suppl 15, S2	3.6	45
89	Comprehensive splicing graph analysis of alternative splicing patterns in chicken, compared to human and mouse. *BMC Genomics*, **2009**, 10 Suppl 1, S5	4.5	18
88	Genome-wide analysis of alternative splicing in cow: implications in bovine as a model for human diseases. *BMC Genomics*, **2009**, 10 Suppl 3, S11	4.5	19
87	A multi-species comparative structural bioinformatics analysis of inherited mutations in alpha-D-mannosidase reveals strong genotype-phenotype correlation. *BMC Genomics*, **2009**, 10 Suppl 3, S33	4.5	8
86	A proposed minimum skill set for university graduates to meet the informatics needs and challenges of the "-omics" era. *BMC Genomics*, **2009**, 10 Suppl 3, S36	4.5	32
85	A multi-factor model for caspase degradome prediction. *BMC Genomics*, **2009**, 10 Suppl 3, S6	4.5	10
84	Improved insights into the transcriptomes of the human hookworm Necator americanus--fundamental and biotechnological implications. *Biotechnology Advances*, **2009**, 27, 122-32	17.8	17

83	Advanced in silico analysis of expressed sequence tag (EST) data for parasitic nematodes of major socio-economic importance--fundamental insights toward biotechnological outcomes. *Biotechnology Advances*, **2009**, 27, 439-48	17.8	28
82	An integrated transcriptomics and proteomics analysis of the secretome of the helminth pathogen Fasciola hepatica: proteins associated with invasion and infection of the mammalian host. *Molecular and Cellular Proteomics*, **2009**, 8, 1891-907	7.6	203
81	The genome sequence of taurine cattle: a window to ruminant biology and evolution. *Science*, **2009**, 324, 522-8	33.3	863
80	Secretome: clues into pathogen infection and clinical applications. *Genome Medicine*, **2009**, 1, 113	14.4	39
79	Structural Immunoinformatics: Understanding MHC-Peptide-TR Binding **2009**, 77-93		0
78	Bioinformatics research in the Asia Pacific: a 2007 update. *BMC Bioinformatics*, **2008**, 9 Suppl 1, S1	3.6	4
77	In silico analysis of expressed sequence tags from Trichostrongylus vitrinus (Nematoda): comparison of the automated ESTExplorer workflow platform with conventional database searches. *BMC Bioinformatics*, **2008**, 9 Suppl 1, S10	3.6	17
76	Modeling Escherichia coli signal peptidase complex with bound substrate: determinants in the mature peptide influencing signal peptide cleavage. *BMC Bioinformatics*, **2008**, 9 Suppl 1, S15	3.6	9
75	Tandem duplication, circular permutation, molecular adaptation: how Solanaceae resist pests via inhibitors. *BMC Bioinformatics*, **2008**, 9 Suppl 1, S22	3.6	25
74	Flanking signal and mature peptide residues influence signal peptide cleavage. *BMC Bioinformatics*, **2008**, 9 Suppl 12, S15	3.6	42
73	CMKb: a web-based prototype for integrating Australian Aboriginal customary medicinal plant knowledge. *BMC Bioinformatics*, **2008**, 9 Suppl 12, S25	3.6	14
72	Gender-enriched transcripts in Haemonchus contortus--predicted functions and genetic interactions based on comparative analyses with Caenorhabditis elegans. *International Journal for Parasitology*, **2008**, 38, 65-83	4.3	36
71	Structural Immunoinformatics **2008**, 51-61		1
70	Functional and structural implications of the complement factor H Y402H polymorphism associated with age-related macular degeneration. *Investigative Ophthalmology and Visual Science*, **2008**, 49, 1763-70		70
69	Transcriptional changes in the hookworm, Ancylostoma caninum, during the transition from a free-living to a parasitic larva. *PLoS Neglected Tropical Diseases*, **2008**, 2, e130	4.8	66
68	Needles in the EST haystack: large-scale identification and analysis of excretory-secretory (ES) proteins in parasitic nematodes using expressed sequence tags (ESTs). *PLoS Neglected Tropical Diseases*, **2008**, 2, e301	4.8	40
67	A practical guide to structure-based prediction of MHC-binding peptides. *Methods in Molecular Biology*, **2007**, 409, 301-8	1.4	5
66	In silico characterization of immunogenic epitopes presented by HLA-Cw*0401. *Immunome Research*, **2007**, 3, 7		13

65	A transcriptomic analysis of the adult stage of the bovine lungworm, Dictyocaulus viviparus. *BMC Genomics*, **2007**, 8, 311	4.5	16
64	Oesophagostomum dentatum: potential as a model for genomic studies of strongylid nematodes, with biotechnological prospects. *Biotechnology Advances*, **2007**, 25, 281-93	17.8	18
63	Methods and protocols for prediction of immunogenic epitopes. *Briefings in Bioinformatics*, **2007**, 8, 96-108	13.4	83
62	A workflow for mutation extraction and structure annotation. *Journal of Bioinformatics and Computational Biology*, **2007**, 5, 1319-37	1	19
61	CASVM: web server for SVM-based prediction of caspase substrates cleavage sites. *Bioinformatics*, **2007**, 23, 3241-3	7.2	61
60	In silico grouping of peptide/HLA class I complexes using structural interaction characteristics. *Bioinformatics*, **2007**, 23, 177-83	7.2	123
59	ESTExplorer: an expressed sequence tag (EST) assembly and annotation platform. *Nucleic Acids Research*, **2007**, 35, W143-7	20.1	56
58	Genomic characterization of Tv-ant-1, a Caenorhabditis elegans tag-61 homologue from the parasitic nematode Trichostrongylus vitrinus. *Gene*, **2007**, 397, 12-25	3.8	8
57	A hitchhiker's guide to expressed sequence tag (EST) analysis. *Briefings in Bioinformatics*, **2007**, 8, 6-21	13.4	200
56	Establishing bioinformatics research in the Asia Pacific. *BMC Bioinformatics*, **2006**, 7, 1	3.6	114
55	SVM-based prediction of caspase substrate cleavage sites. *BMC Bioinformatics*, **2006**, 7 Suppl 5, S14	3.6	48
54	Prediction of desmoglein-3 peptides reveals multiple shared T-cell epitopes in HLA DR4- and DR6-associated pemphigus vulgaris. *BMC Bioinformatics*, **2006**, 7 Suppl 5, S7	3.6	20
53	ASGS: an alternative splicing graph web service. *Nucleic Acids Research*, **2006**, 34, W444-7	20.1	13
52	Prediction of HLA-DQ3.2beta ligands: evidence of multiple registers in class II binding peptides. *Bioinformatics*, **2006**, 22, 1232-8	7.2	38
51	Comparative Genomic Analysis of Glycoylation Pathways in Yeast, Plants and Higher eukaryotes. *Applied Mycology and Biotechnology*, **2006**, 6, 227-248		2
50	MPID-T: database for sequence-structure-function information on T-cell receptor/peptide/MHC interactions. *Applied Bioinformatics*, **2006**, 5, 111-4		22
49	SCORPION2: a database for structure-function analysis of scorpion toxins. *Toxicon*, **2006**, 47, 356-63	2.8	45
48	OMIA (Online Mendelian Inheritance in Animals): an enhanced platform and integration into the Entrez search interface at NCBI. *Nucleic Acids Research*, **2006**, 34, D599-601	20.1	59

47	Modeling the bound conformation of Pemphigus vulgaris-associated peptides to MHC Class II DR and DQ alleles. *Immunome Research*, **2006**, 2, 1		71
46	Deduction of functional peptide motifs in scorpion toxins. *Journal of Peptide Science*, **2006**, 12, 420-7	2.1	9
45	Cloning and molecular characterization of the first aquatic hyaluronidase, SFHYA1, from the venom of stonefish (Synanceja horrida). *Gene*, **2005**, 346, 71-81	3.8	23
44	Accurate prediction of scorpion toxin functional properties from primary structures. *Journal of Molecular Graphics and Modelling*, **2005**, 24, 17-24	2.8	12
43	SPdb--a signal peptide database. *BMC Bioinformatics*, **2005**, 6, 249	3.6	71
42	Bioinformatics education--perspectives and challenges. *PLoS Computational Biology*, **2005**, 1, e52	5	43
41	The integrin alpha L beta 2 hybrid domain serves as a link for the propagation of activation signal from its stalk regions to the I-like domain. *Journal of Biological Chemistry*, **2004**, 279, 54334-9	5.4	25
40	SDPMOD: an automated comparative modeling server for small disulfide-bonded proteins. *Nucleic Acids Research*, **2004**, 32, W356-9	20.1	17
39	Delineation of modular proteins: domain boundary prediction from sequence information. *Briefings in Bioinformatics*, **2004**, 5, 179-92	13.4	24
38	DEDB: a database of Drosophila melanogaster exons in splicing graph form. *BMC Bioinformatics*, **2004**, 5, 189	3.6	23
37	Xpro: database of eukaryotic protein-encoding genes. *Nucleic Acids Research*, **2004**, 32, D59-63	20.1	17
36	Modeling the structure of bound peptide ligands to major histocompatibility complex. *Protein Science*, **2004**, 13, 2523-32	6.3	70
35	XdomView: protein domain and exon position visualization. *Bioinformatics*, **2003**, 19, 159-60	7.2	9
34	A common site within factor H SCR 7 responsible for binding heparin, C-reactive protein and streptococcal M protein. *European Journal of Immunology*, **2003**, 33, 962-9	6.1	143
33	The S-star trial bioinformatics course: An on-line learning success*. *Biochemistry and Molecular Biology Education*, **2003**, 31, 20-23	1.3	15
32	MGAlignIt: A web service for the alignment of mRNA/EST and genomic sequences. *Nucleic Acids Research*, **2003**, 31, 3533-6	20.1	28
31	MPID: MHC-Peptide Interaction Database for sequence-structure-function information on peptides binding to MHC molecules. *Bioinformatics*, **2003**, 19, 309-10	7.2	31
30	Antisense Suppression of a Cytokinin-binding Protein from Petunia Causes Excessive Branching and Reduces Adventitious Shoot Bud Induction in Vitro **2003**, 285-287		

29	kappa-Hefutoxin1, a novel toxin from the scorpion Heterometrus fulvipes with unique structure and function. Importance of the functional diad in potassium channel selectivity. *Journal of Biological Chemistry*, **2002**, 277, 30040-7	5.4	114
28	APBioNet: the Asia-Pacific regional consortium for bioinformatics. *Applied Bioinformatics*, **2002**, 1, 101-5		5
27	The hand, foot and mouth disease virus capsid: sequence analysis and prediction of antigenic sites from homology modelling. *Applied Bioinformatics*, **2002**, 1, 43-52		23
26	Multiple ligand binding sites on domain seven of human complement factor H. *International Immunopharmacology*, **2001**, 1, 433-43	5.8	38
25	Molecular modeling on the Web. *BioTechniques*, **2001**, 30, 50-2	2.5	6
24	The gene for a novel member of the whey acidic protein family encodes three four-disulfide core domains and is asynchronously expressed during lactation. *Journal of Biological Chemistry*, **2000**, 275, 23074-81	5.4	67
23	Complement factor H: sequence analysis of 221 kb of human genomic DNA containing the entire fH, fHR-1 and fHR-3 genes. *Molecular Immunology*, **2000**, 37, 41-52	4.3	52
22	Functional and structural studies of wild type SOX9 and mutations causing campomelic dysplasia. *Journal of Biological Chemistry*, **1999**, 274, 24023-30	5.4	85
21	The whey acidic protein family: a new signature motif and three-dimensional structure by comparative modeling. *Journal of Molecular Graphics and Modelling*, **1999**, 17, 106-13, 134-6	2.8	111
20	Hybrid Quantum and Molecular Mechanical (QM/MM) Studies on the Pyruvate to l-Lactate Interconversion in l-Lactate Dehydrogenase. *Journal of Physical Chemistry B*, **1997**, 101, 5614-5618	3.4	53
19	Predicted structure of the extracellular region of ligand-gated ion-channel receptors shows SH2-like and SH3-like domains forming the ligand-binding site. *Protein Science*, **1997**, 6, 983-98	6.3	32
18	Mechanistic aspects of biological redox reactions involving NADH. Part 5.AM1 transition-state studies for the pyruvate⊡-lactate interconversion in L-lactate dehydrogenase. *Journal of the Chemical Society, Faraday Transactions*, **1994**, 90, 2047-2056		17
17	Substituent effects on carbonyl bond orders. *Computational and Theoretical Chemistry*, **1991**, 233, 83-87		
16	Radial behavior of the average local ionization energies of atoms. *Journal of Chemical Physics*, **1991**, 95, 6699-6704	3.9	82
15	Correlations between the solvent hydrogen bond acceptor parameter .beta. and the calculated molecular electrostatic potential. *Journal of Organic Chemistry*, **1991**, 56, 3734-3737	4.2	106
14	A computational analysis of the electrostatic potentials and relative bond strengths of hydrazine and some of its 1,1-dimethyl derivatives. *International Journal of Quantum Chemistry*, **1990**, 37, 611-629	2.1	8
13	Computational evaluation and comparison of some nitramine properties. *Journal of the American Chemical Society*, **1988**, 110, 3425-3430	16.4	46
12	Bond-order-bond-energy correlations. *Chemical Physics Letters*, **1986**, 124, 527-530	2.5	46

11	Compliant fields for molecular interactions: Water dimer and formic acid dimer. *International Journal of Quantum Chemistry*, **1985**, 27, 547-557	2.1	1
10	The gramicidin A channel: theoretical energy profile computed for single occupancy by a divalent cation, Ca2+. *Biochimica Et Biophysica Acta - Biomembranes*, **1985**, 818, 23-30	3.8	12
9	An ab initio study of the binding of N2 to Na+ and K+. *Chemical Physics Letters*, **1984**, 110, 346-350	2.5	12
8	Ab initio study of the stepwise hydration of NO+. *Chemical Physics Letters*, **1984**, 107, 107-111	2.5	18
7	The gramicidin A channel: comparison of the energy profiles of Na+, K+ and Cs+. Influence of the flexibility of the ethanolamine end chain on the profiles. *FEBS Letters*, **1984**, 173, 301-6	3.8	35
6	The use of CNDO/force and compliance constant methods in evaluating quadratic potential functions of carbonyl and formyl fluorides. *Journal of Computational Chemistry*, **1983**, 4, 175-180	3.5	3
5	Compliant fields for formic acid and formamide. *Journal of the Chemical Society, Faraday Transactions 2*, **1983**, 79, 1699		2
4	Compliant fields for water, ammonia and methane. *Computational and Theoretical Chemistry*, **1983**, 104, 1-8		3
3	The force field of carbon suboxide. *Computational and Theoretical Chemistry*, **1982**, 90, 219-226		3
2	The force field of carbon suboxide. *Journal of Molecular Structure*, **1982**, 90, 219-226	3.4	1
1	Semiempirical molecular-orbital studies on the problem of nonclassical resonance in the homoallylic cation. *International Journal of Quantum Chemistry*, **1980**, 18, 1479-1482	2.1	1