Philip E Bourne

List of Publications by Year in Descending Order

204 papers	41,921 citations	61 h-index	204 g-index
279 ext. papers	49,875 ext. citations	7.7 avg, IF	6.99 L-index

#	Paper	IF	Citations
204	Is "bioinformatics" dead?. *PLoS Biology*, **2021**, 19, e3001165	9.7	4
203	IL-13 is a driver of COVID-19 severity. *JCI Insight*, **2021**, 6,	9.9	18
202	Informatics-enabled citizen science to advance health equity. *Journal of the American Medical Informatics Association: JAMIA*, **2021**, 28, 2009-2012	8.6	1
201	Real-world evidence for improved outcomes with histamine antagonists and aspirin in 22,560 COVID-19 patients. *Signal Transduction and Targeted Therapy*, **2021**, 6, 267	21	5
200	A Birds-Eye (Re)View of Acid-Suppression Drugs, COVID-19, and the Highly Variable Literature. *Frontiers in Pharmacology*, **2021**, 12, 700703	5.6	3
199	Computational Prediction of Potential Inhibitors of the Main Protease of SARS-CoV-2. *Frontiers in Chemistry*, **2020**, 8, 590263	5	12
198	Revealing Acquired Resistance Mechanisms of Kinase-Targeted Drugs Using an on-the-Fly, Function-Site Interaction Fingerprint Approach. *Journal of Chemical Theory and Computation*, **2020**, 16, 3152-3161	6.4	3
197	Overview of Current Type I/II Kinase Inhibitors **2020**, 13-28		1
196	Structural Insights into the Binding Modes of Viral RNA-Dependent RNA Polymerases Using a Function-Site Interaction Fingerprint Method for RNA Virus Drug Discovery. *Journal of Proteome Research*, **2020**, 19, 4698-4705	5.6	9
195	Evidence for treatment with estradiol for women with SARS-CoV-2 infection. *BMC Medicine*, **2020**, 18, 369	11.4	53
194	Ten simple rules for writing scientific op-ed articles. *PLoS Computational Biology*, **2020**, 16, e1008187	5	1
193	Analyzing the symmetrical arrangement of structural repeats in proteins with CE-Symm. *PLoS Computational Biology*, **2019**, 15, e1006842	5	13
192	Natural language processing of symptoms documented in free-text narratives of electronic health records: a systematic review. *Journal of the American Medical Informatics Association: JAMIA*, **2019**, 26, 364-379	8.6	112
191	The Urfold: Structural similarity just above the superfold level?. *Protein Science*, **2019**, 28, 2119-2126	6.3	4
190	A systematic review of natural language processing and text mining of symptoms from electronic patient-authored text data. *International Journal of Medical Informatics*, **2019**, 125, 37-46	5.3	65
189	Translational Health Disparities Research in a Data-Rich World. *Health Equity*, **2019**, 3, 588-600	3.1	15
188	Structural Insights into Characterizing Binding Sites in Epidermal Growth Factor Receptor Kinase Mutants. *Journal of Chemical Information and Modeling*, **2019**, 59, 453-462	6.1	13

187	The Small β-Barrel Domain: A Survey-Based Structural Analysis. *Structure*, **2019**, 27, 6-26	5.2	15
186	Progress with covalent small-molecule kinase inhibitors. *Drug Discovery Today*, **2018**, 23, 727-735	8.8	120
185	Cloud computing applications for biomedical science: A perspective. *PLoS Computational Biology*, **2018**, 14, e1006144	5	42
184	Structural biology meets data science: does anything change?. *Current Opinion in Structural Biology*, **2018**, 52, 95-102	8.1	5
183	Determining Cysteines Available for Covalent Inhibition Across the Human Kinome. *Journal of Medicinal Chemistry*, **2017**, 60, 2879-2889	8.3	66
182	Insights into the binding mode of MEK type-III inhibitors. A step towards discovering and designing allosteric kinase inhibitors across the human kinome. *PLoS ONE*, **2017**, 12, e0179936	3.7	22
181	BioJava-ModFinder: identification of protein modifications in 3D structures from the Protein Data Bank. *Bioinformatics*, **2017**, 33, 2047-2049	7.2	8
180	Should biomedical research be like Airbnb?. *PLoS Biology*, **2017**, 15, e2001818	9.7	2
179	Big Data Science: Opportunities and Challenges to Address Minority Health and Health Disparities in the 21st Century. *Ethnicity and Disease*, **2017**, 27, 95-106	1.8	81
178	Harnessing Big Data for Systems Pharmacology. *Annual Review of Pharmacology and Toxicology*, **2017**, 57, 245-262	17.9	45
177	Developing international open science collaborations: Funder reflections on the Open Science Prize. *PLoS Biology*, **2017**, 15, e2002617	9.7	1
176	Building the biomedical data science workforce. *PLoS Biology*, **2017**, 15, e2003082	9.7	16
175	Life is three-dimensional, and it begins with molecules. *PLoS Biology*, **2017**, 15, e2002041	9.7	1
174	Systems biology of the structural proteome. *BMC Systems Biology*, **2016**, 10, 26	3.5	39
173	Drug repurposing to target Ebola virus replication and virulence using structural systems pharmacology. *BMC Bioinformatics*, **2016**, 17, 90	3.6	41
172	Author response: How open science helps researchers succeed **2016**,		9
171	How open science helps researchers succeed. *ELife*, **2016**, 5,	8.9	280
170	The FAIR Guiding Principles for scientific data management and stewardship. *Scientific Data*, **2016**, 3, 160018	8.2	4154

169	SCIENTIFIC COMMUNITY. Preprints for the life sciences. *Science*, **2016**, 352, 899-901	33.3	68
168	Delineation of Polypharmacology across the Human Structural Kinome Using a Functional Site Interaction Fingerprint Approach. *Journal of Medicinal Chemistry*, **2016**, 59, 4326-41	8.3	31
167	Toward effective software solutions for big biology. *Nature Biotechnology*, **2015**, 33, 686-7	44.5	25
166	The RCSB Protein Data Bank: views of structural biology for basic and applied research and education. *Nucleic Acids Research*, **2015**, 43, D345-56	20.1	375
165	Perspective: Sustaining the big-data ecosystem. *Nature*, **2015**, 527, S16-7	50.4	74
164	Zeta Inhibitory Peptide Disrupts Electrostatic Interactions That Maintain Atypical Protein Kinase C in Its Active Conformation on the Scaffold p62. *Journal of Biological Chemistry*, **2015**, 290, 21845-56	5.4	22
163	The NIH Big Data to Knowledge (BD2K) initiative. *Journal of the American Medical Informatics Association: JAMIA*, **2015**, 22, 1114	8.6	51
162	Let's Make Gender Diversity in Data Science a Priority Right from the Start. *PLoS Biology*, **2015**, 13, e1002206	9.7	5
161	Developing multi-target therapeutics to fine-tune the evolutionary dynamics of the cancer ecosystem. *Frontiers in Pharmacology*, **2015**, 6, 209	5.6	30
160	DOIs for DICOM raw images: enabling science reproducibility. *Radiology*, **2015**, 275, 3-4	20.5	4
159	RCSB PDB Mobile: iOS and Android mobile apps to provide data access and visualization to the RCSB Protein Data Bank. *Bioinformatics*, **2015**, 31, 126-7	7.2	9
158	Detection of circular permutations within protein structures using CE-CP. *Bioinformatics*, **2015**, 31, 1316-8	7.2	8
157	Achievements and challenges in structural bioinformatics and computational biophysics. *Bioinformatics*, **2015**, 31, 146-50	7.2	20
156	Combinatorial approach for large-scale identification of linked peptides from tandem mass spectrometry spectra. *Molecular and Cellular Proteomics*, **2014**, 13, 1128-36	7.6	17
155	A turn-key approach for large-scale identification of complex posttranslational modifications. *Journal of Proteome Research*, **2014**, 13, 1190-9	5.6	5
154	Systematic detection of internal symmetry in proteins using CE-Symm. *Journal of Molecular Biology*, **2014**, 426, 2255-68	6.5	35
153	MixGF: spectral probabilities for mixture spectra from more than one peptide. *Molecular and Cellular Proteomics*, **2014**, 13, 3688-97	7.6	15
152	Towards structural systems pharmacology to study complex diseases and personalized medicine. *PLoS Computational Biology*, **2014**, 10, e1003554	5	47

151	Anti-infectious drug repurposing using an integrated chemical genomics and structural systems biology approach. *Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing*, **2014**, 136-47	1.3	9
150	Multiscale modeling of the causal functional roles of nsSNPs in a genome-wide association study: application to hypoxia. *BMC Genomics*, **2013**, 14 Suppl 3, S9	4.5	6
149	Antibacterial mechanisms identified through structural systems pharmacology. *BMC Systems Biology*, **2013**, 7, 102	3.5	20
148	Communication of scientific information: is it time to reassess?. *Clinical Chemistry*, **2013**, 59, 604-11	5.5	1
147	Biodiversity data should be published, cited, and peer reviewed. *Trends in Ecology and Evolution*, **2013**, 28, 454-61	10.9	157
146	ANTI-INFECTIOUS DRUG REPURPOSING USING AN INTEGRATED CHEMICAL GENOMICS AND STRUCTURAL SYSTEMS BIOLOGY APPROACH **2013**,		2
145	The reaming of life: based on the 2010 Jim Gray eScience Award Lecture. *Concurrency Computation Practice and Experience*, **2013**, 25, 445-453	1.4	0
144	Quantifying reproducibility in computational biology: the case of the tuberculosis drugome. *PLoS ONE*, **2013**, 8, e80278	3.7	69
143	The RCSB Protein Data Bank: new resources for research and education. *Nucleic Acids Research*, **2013**, 41, D475-82	20.1	371
142	Immune epitope database analysis resource. *Nucleic Acids Research*, **2012**, 40, W525-30	20.1	322
141	Raloxifene attenuates Pseudomonas aeruginosa pyocyanin production and virulence. *International Journal of Antimicrobial Agents*, **2012**, 40, 246-51	14.3	65
140	Receptor databases and computational websites for ligand binding. *Methods in Molecular Biology*, **2012**, 897, 1-13	1.4	4
139	Predicting the Polypharmacology of Drugs: Identifying New Uses through Chemoinformatics, Structural Informatics, and Molecular Modeling-Based Approaches **2012**, 163-205		4
138	Novel computational approaches to polypharmacology as a means to define responses to individual drugs. *Annual Review of Pharmacology and Toxicology*, **2012**, 52, 361-79	17.9	168
137	SuperTarget goes quantitative: update on drug-target interactions. *Nucleic Acids Research*, **2012**, 40, D1113-7	20.1	139
136	BioJava: an open-source framework for bioinformatics in 2012. *Bioinformatics*, **2012**, 28, 2693-5	7.2	136
135	Discrepancies in purified and cellular PKMζ inhibition profiles invalidate its proposed role as a mediator of memory. *FASEB Journal*, **2012**, 26, 768.5	0.9	
134	Drug discovery using chemical systems biology: weak inhibition of multiple kinases may contribute to the anti-cancer effect of nelfinavir. *PLoS Computational Biology*, **2011**, 7, e1002037	5	126

133	A machine learning-based method to improve docking scoring functions and its application to drug repurposing. *Journal of Chemical Information and Modeling*, **2011**, 51, 408-19	6.1	138
132	Peptide identification by database search of mixture tandem mass spectra. *Molecular and Cellular Proteomics*, **2011**, 10, M111.010017	7.6	23
131	Institutional Profile: University of California San Diego Pharmacogenomics Education Program (PharmGenEd): bridging the gap between science and practice. *Pharmacogenomics*, **2011**, 12, 149-53	2.6	23
130	Structure-based systems biology for analyzing off-target binding. *Current Opinion in Structural Biology*, **2011**, 21, 189-99	8.1	116
129	The evolution of the RCSB Protein Data Bank website. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 782-789	7.9	6
128	The origin of a derived superkingdom: how a gram-positive bacterium crossed the desert to become an archaeon. *Biology Direct*, **2011**, 6, 16	7.2	26
127	IEDB-3D: structural data within the immune epitope database. *Nucleic Acids Research*, **2011**, 39, D1164-70	20.1	42
126	Coarse-graining the electrostatic potential via distributed multipole expansions. *Computer Physics Communications*, **2011**, 182, 1455-1462	4.2	3
125	PROMISCUOUS: a database for network-based drug-repositioning. *Nucleic Acids Research*, **2011**, 39, D1060-6	20.1	172
124	The RCSB Protein Data Bank: redesigned web site and web services. *Nucleic Acids Research*, **2011**, 39, D392-401	20.1	461
123	Cobweb: a Java applet for network exploration and visualisation. *Bioinformatics*, **2011**, 27, 1725-6	7.2	7
122	Quality assurance for the query and distribution systems of the RCSB Protein Data Bank. *Database: the Journal of Biological Databases and Curation*, **2011**, 2011, bar003	5	6
121	Digital research/analog publishing: one scientist's view. *Serials*, **2011**, 24, 119-122		
120	SMAP-WS: a parallel web service for structural proteome-wide ligand-binding site comparison. *Nucleic Acids Research*, **2010**, 38, W441-4	20.1	53
119	A multidimensional strategy to detect polypharmacological targets in the absence of structural and sequence homology. *PLoS Computational Biology*, **2010**, 6, e1000648	5	61
118	What do I want from the publisher of the future?. *PLoS Computational Biology*, **2010**, 6, e1000787	5	15
117	Drug off-target effects predicted using structural analysis in the context of a metabolic network model. *PLoS Computational Biology*, **2010**, 6, e1000938	5	165
116	Will widgets and semantic tagging change computational biology?. *PLoS Computational Biology*, **2010**, 6, e1000673	5	7

115	The Mycobacterium tuberculosis drugome and its polypharmacological implications. *PLoS Computational Biology*, **2010**, 6, e1000976	5	82
114	Pre-calculated protein structure alignments at the RCSB PDB website. *Bioinformatics*, **2010**, 26, 2983-5	7.2	156
113	History of biological metal utilization inferred through phylogenomic analysis of protein structures. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 10567-72	11.5	210
112	Integration of open access literature into the RCSB Protein Data Bank using BioLit. *BMC Bioinformatics*, **2010**, 11, 220	3.6	7
111	dConsensus: a tool for displaying domain assignments by multiple structure-based algorithms and for construction of a consensus assignment. *BMC Bioinformatics*, **2010**, 11, 310	3.6	14
110	Save the tree of life or get lost in the woods. *Biology Direct*, **2010**, 5, 44	7.2	7
109	Genome Evolution Studied Through Protein Structure **2010**, 153-164		1
108	Limitations of Ab initio predictions of peptide binding to MHC class II molecules. *PLoS ONE*, **2010**, 5, e9232	3.7	39
107	A unified statistical model to support local sequence order independent similarity searching for ligand-binding sites and its application to genome-based drug discovery. *Bioinformatics*, **2009**, 25, i305-12	7.2	76
106	Drug discovery using chemical systems biology: identification of the protein-ligand binding network to explain the side effects of CETP inhibitors. *PLoS Computational Biology*, **2009**, 5, e1000387	5	200
105	Nothing about protein structure classification makes sense except in the light of evolution. *Current Opinion in Structural Biology*, **2009**, 19, 329-34	8.1	29
104	Structural analysis of polarizing indels: an emerging consensus on the root of the tree of life. *Biology Direct*, **2009**, 4, 30	7.2	27
103	Drug discovery using chemical systems biology: repositioning the safe medicine Comtan to treat multi-drug and extensively drug resistant tuberculosis. *PLoS Computational Biology*, **2009**, 5, e1000423	5	234
102	The evolutionary history of protein domains viewed by species phylogeny. *PLoS ONE*, **2009**, 4, e8378	3.7	63
101	ElliPro: a new structure-based tool for the prediction of antibody epitopes. *BMC Bioinformatics*, **2008**, 9, 514	3.6	667
100	Immune epitope database analysis resource (IEDB-AR). *Nucleic Acids Research*, **2008**, 36, W513-8	20.1	240
99	Superimpose: a 3D structural superposition server. *Nucleic Acids Research*, **2008**, 36, W47-54	20.1	30
98	Detecting evolutionary relationships across existing fold space, using sequence order-independent profile-profile alignments. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 5441-6	11.5	209

97	Computational biology resources lack persistence and usability. *PLoS Computational Biology*, **2008**, 4, e1000136	5	23
96	BioLit: integrating biological literature with databases. *Nucleic Acids Research*, **2008**, 36, W385-9	20.1	26
95	I am not a scientist, I am a number. *PLoS Computational Biology*, **2008**, 4, e1000247	5	8
94	Resolving a distribution of charge into intrinsic multipole moments: a rankwise distributed multipole analysis. *Physical Review E*, **2008**, 78, 066601	2.4	3
93	Rethinking proteasome evolution: two novel bacterial proteasomes. *Journal of Molecular Evolution*, **2008**, 66, 494-504	3.1	26
92	SuperTarget and Matador: resources for exploring drug-target relationships. *Nucleic Acids Research*, **2008**, 36, D919-22	20.1	416
91	Analysis of the human kinome using methods including fold recognition reveals two novel kinases. *PLoS ONE*, **2008**, 3, e1597	3.7	9
90	Intrinsic evaluation of text mining tools may not predict performance on realistic tasks. *Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing*, **2008**, 640-51	1.3	20
89	Antibody-protein interactions: benchmark datasets and prediction tools evaluation. *BMC Structural Biology*, **2007**, 7, 64	2.7	151
88	EpitopeViewer: a Java application for the visualization and analysis of immune epitopes in the Immune Epitope Database and Analysis Resource (IEDB). *Immunome Research*, **2007**, 3, 3		37
87	High-throughput identification of interacting protein-protein binding sites. *BMC Bioinformatics*, **2007**, 8, 223	3.6	8
86	A robust and efficient algorithm for the shape description of protein structures and its application in predicting ligand binding sites. *BMC Bioinformatics*, **2007**, 8 Suppl 4, S9	3.6	96
85	In silico elucidation of the molecular mechanism defining the adverse effect of selective estrogen receptor modulators. *PLoS Computational Biology*, **2007**, 3, e217	5	70
84	Con-Struct Map: a comparative contact map analysis tool. *Bioinformatics*, **2007**, 23, 2491-2	7.2	10
83	INTRINSIC EVALUATION OF TEXT MINING TOOLS MAY NOT PREDICT PERFORMANCE ON REALISTIC TASKS **2007**,		4
82	Outcome of a workshop on archiving structural models of biological macromolecules. *Structure*, **2006**, 14, 1211-7	5.2	49
81	The RCSB PDB information portal for structural genomics. *Nucleic Acids Research*, **2006**, 34, D302-5	20.1	249
80	Wiggle-predicting functionally flexible regions from primary sequence. *PLoS Computational Biology*, **2006**, 2, e90	5	25

79	Modern proteomes contain putative imprints of ancient shifts in trace metal geochemistry. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 17822-7	11.5	182
78	Partitioning protein structures into domains: why is it so difficult?. *Journal of Molecular Biology*, **2006**, 361, 562-90	6.5	88
77	Exploiting sequence and structure homologs to identify protein-protein binding sites. *Proteins: Structure, Function and Bioinformatics*, **2006**, 62, 630-40	4.2	67
76	Structure Comparison and Alignment. *Methods of Biochemical Analysis*, **2005**, 321-337		1
75	Inferring Protein Function from Structure. *Methods of Biochemical Analysis*, **2005**, 387-407		3
74	Defining Bioinformatics and Structural Bioinformatics. *Methods of Biochemical Analysis*, **2005**, 1-14		2
73	Fundamentals of Protein Structure. *Methods of Biochemical Analysis*, **2005**, 15-39		2
72	Fundamentals of DNA and RNA Structure. *Methods of Biochemical Analysis*, **2005**, 41-73		1
71	Macromolecular Structure Determination by NMR Spectroscopy. *Methods of Biochemical Analysis*, **2005**, 89-113		3
70	Molecular Visualization. *Methods of Biochemical Analysis*, **2005**, 135-158		1
69	The PDB Format, mmCIF Formats, and Other Data Formats. *Methods of Biochemical Analysis*, **2005**, 159-179		9
68	The Protein Data Bank. *Methods of Biochemical Analysis*, **2005**, 181-198		3
67	The Nucleic Acid Database. *Methods of Biochemical Analysis*, **2005**, 199-216		1
66	Other Structure-Based Databases. *Methods of Biochemical Analysis*, **2005**, 217-236		
65	Protein Structure Evolution and the Scop Database. *Methods of Biochemical Analysis*, **2005**, 237-248		0
64	The RCSB Protein Data Bank: a redesigned query system and relational database based on the mmCIF schema. *Nucleic Acids Research*, **2005**, 33, D233-7	20.1	259
63	Structural Genomics. *Methods of Biochemical Analysis*, **2005**, 589-612		2
62	All-Atom Contacts: A New Approach to Structure Validation. *Methods of Biochemical Analysis*, **2005**, 305-320		1

61	Identifying Structural Domains in Proteins. *Methods of Biochemical Analysis*, **2005**, 365-385		3
60	Structural Quality Assurance. *Methods of Biochemical Analysis*, **2005**, 273-303		11
59	Secondary Structure Assignment. *Methods of Biochemical Analysis*, **2005**, 339-363		3
58	Prediction of Protein-Protein Interactions from Evolutionary Information. *Methods of Biochemical Analysis*, **2005**, 409-426		4
57	CASP and CAFASP Experiments and Their Findings. *Methods of Biochemical Analysis*, **2005**, 499-507		2
56	Prediction in 1D: Secondary Structure, Membrane Helices, and Accessibility. *Methods of Biochemical Analysis*, **2005**, 559-587		7
55	The Molecular Biology Toolkit (MBT): a modular platform for developing molecular visualization applications. *BMC Bioinformatics*, **2005**, 6, 21	3.6	227
54	An ontology for immune epitopes: application to the design of a broad scope database of immune reactivities. *Immunome Research*, **2005**, 1, 2		32
53	Assigning new GO annotations to protein data bank sequences by combining structure and sequence homology. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 855-65	4.2	18
52	Structural evolution of the protein kinase-like superfamily. *PLoS Computational Biology*, **2005**, 1, e49	5	191
51	Functional coverage of the human genome by existing structures, structural genomics targets, and homology models. *PLoS Computational Biology*, **2005**, 1, e31	5	51
50	Will a biological database be different from a biological journal?. *PLoS Computational Biology*, **2005**, 1, 179-81	5	65
49	Overview of Structural Bioinformatics **2005**, 15-44		
48	Principles and Methods of Docking and Ligand Design. *Methods of Biochemical Analysis*, **2005**, 441-476		2
47	Electrostatic Interactions. *Methods of Biochemical Analysis*, **2005**, 427-440		4
46	Phylogeny determined by protein domain content. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 373-8	11.5	174
45	Structural Evolution of the Protein Kinase-Like Superfamily. *PLoS Computational Biology*, **2005**, preprint, e49	5	3
44	Functional Coverage of the Human Genome by Existing Structures, Structural Genomics Targets and Homology Models. *PLoS Computational Biology*, **2005**, preprint, e31	5	

43	In Silico Elucidation of the Molecular Mechanism Defining the Adverse Effect of Selective Estrogen Receptor Modulators. *PLoS Computational Biology*, **2005**, preprint, e217	5	
42	A new scoring function and associated statistical significance for structure alignment by CE. *Journal of Computational Biology*, **2004**, 11, 787-99	1.7	20
41	The Protein Data Bank and lessons in data management. *Briefings in Bioinformatics*, **2004**, 5, 23-30	13.4	16
40	Statistical and visual morph movie analysis of crystallographic mutant selection bias in protein mutation resource data. *Journal of Bioinformatics and Computational Biology*, **2004**, 2, 61-75	1	2
39	CE-MC: a multiple protein structure alignment server. *Nucleic Acids Research*, **2004**, 32, W100-3	20.1	85
38	The distribution and query systems of the RCSB Protein Data Bank. *Nucleic Acids Research*, **2004**, 32, D223-5	20.1	95
37	The encyclopedia of life project: Grid software and deployment. *New Generation Computing*, **2004**, 22, 127-136	0.9	14
36	Protein Data Resources **2004**, 478-483		
35	Structural bioinformatics in drug discovery. *Methods of Biochemical Analysis*, **2003**, 44, 477-97		8
34	Computational aspects of high-throughput crystallographic macromolecular structure determination. *Methods of Biochemical Analysis*, **2003**, 44, 75-87		1
33	The Protein Data Bank **2003**, 389-405		24
32	A comparative proteomics resource: proteins of Arabidopsis thaliana. *Genome Biology*, **2003**, 4, R51	18.3	19
31	Ab initio methods. *Methods of Biochemical Analysis*, **2003**, 44, 547-57		7
30	The CATH domain structure database. *Methods of Biochemical Analysis*, **2003**, 44, 249-71		39
29	Fold recognition methods. *Methods of Biochemical Analysis*, **2003**, 44, 525-46		58
28	Homology modeling. *Methods of Biochemical Analysis*, **2003**, 44, 509-23		88
27	Structure comparison and alignment. *Methods of Biochemical Analysis*, **2003**, 44, 321-37		2
26	CASP and CAFASP experiments and their findings. *Methods of Biochemical Analysis*, **2003**, 44, 501-7		13

25	The Protein Data Bank. *Acta Crystallographica Section D: Biological Crystallography*, **2002**, 58, 899-907		1553
24	Protein structure resources. *Acta Crystallographica Section D: Biological Crystallography*, **2002**, 58, 908-15		14
23	The Protein Data Bank: unifying the archive. *Nucleic Acids Research*, **2002**, 30, 245-8	20.1	208
22	Conserved key amino acid positions (CKAAPs) derived from the analysis of common substructures in proteins. *Proteins: Structure, Function and Bioinformatics*, **2001**, 42, 148-63	4.2	34
21	Design and implementation of a collaborative molecular graphics environment. *Journal of Molecular Graphics and Modelling*, **2001**, 19, 280-7, 369-73	2.8	8
20	Announcement of the BioSync web site. *Nature Structural Biology*, **2001**, 8, 663		7
19	CKAAPs DB: a conserved key amino acid positions database. *Nucleic Acids Research*, **2001**, 29, 329-31	20.1	4
18	An alternative view of protein fold space. *Proteins: Structure, Function and Bioinformatics*, **2000**, 38, 247-260	4.2	78
17	The Protein Data Bank and the challenge of structural genomics. *Nature Structural Biology*, **2000**, 7 Suppl, 957-9		424
16	STAR/mmCIF: an ontology for macromolecular structure. *Bioinformatics*, **2000**, 16, 159-68	7.2	67
15	The Protein Data Bank. *Nucleic Acids Research*, **2000**, 28, 235-42	20.1	24073
14	Development of Internet-based multimedia applications. *Trends in Biochemical Sciences*, **1999**, 24, 321-4	10.3	2
13	Macromolecular structure databases: past progress and future challenges. *Acta Crystallographica Section D: Biological Crystallography*, **1998**, 54, 1085-94		3
12	Macromolecular Crystallographic Information File. *Methods in Enzymology*, **1997**, 277, 571-90	1.7	111
11	The protein kinase resource. *Trends in Biochemical Sciences*, **1997**, 22, 444-6	10.3	89
10	A CPU benchmark for protein crystallographic refinement. *Computers in Biology and Medicine*, **1990**, 20, 219-30	7	1
9	Selecting a processor for computations in molecular biophysics. *Computers in Biology and Medicine*, **1988**, 18, 341-9	7	2
8	PRONUC: a software package for the analysis of protein and nucleic acid sequences. *Computer Methods and Programs in Biomedicine*, **1987**, 24, 27-36	6.9	2

List of Publications

7	Structure of a potent neuromuscular blocking agent: Caracurine-II dimethochloride octahydrate, [C40H44N4O2]2+□2Cl□8H2O. *Journal of Crystallographic and Spectroscopic Research*, **1985**, 15, 453-471		4
6	Erabutoxin b. Initial protein refinement and sequence analysis at 0.140-nm resolution. *FEBS Journal*, **1985**, 153, 521-7		42
5	The structure and heavy-metal-ion-binding sites of horse spleen apoferritin. *Biochemical Society Transactions*, **1980**, 8, 654-5	5.1	4
4	The New Biology and the Grid907-922		3
3	Insights into the binding mode of MEK type-III inhibitors. A step towards discovering and designing allosteric kinase inhibitors across the human kinome		1
2	The Small □barrel Domain: A Survey-based Structural Analysis		1
1	Analyzing the symmetrical arrangement of structural repeats in proteins with CE-Symm		1