Tom Blundell

List of Publications by Citations

295 papers	36,152 citations	86 h-index	188 g-index
334 ext. papers	40,151 ext. citations	11.1 avg, IF	7.4 L-index

#	Paper	IF	Citations
295	Comparative protein modelling by satisfaction of spatial restraints. *Journal of Molecular Biology*, **1993**, 234, 779-815	6.5	10363
294	FUGUE: sequence-structure homology recognition using environment-specific substitution tables and structure-dependent gap penalties. *Journal of Molecular Biology*, **2001**, 310, 243-57	6.5	1102
293	pkCSM: Predicting Small-Molecule Pharmacokinetic and Toxicity Properties Using Graph-Based Signatures. *Journal of Medicinal Chemistry*, **2015**, 58, 4066-72	8.3	1056
292	The TRANSPARENT TESTA GLABRA1 locus, which regulates trichome differentiation and anthocyanin biosynthesis in Arabidopsis, encodes a WD40 repeat protein. *Plant Cell*, **1999**, 11, 1337-50	11.6	724
291	Crystal structure of fibroblast growth factor receptor ectodomain bound to ligand and heparin. *Nature*, **2000**, 407, 1029-34	50.4	659
290	Knowledge-based prediction of protein structures and the design of novel molecules. *Nature*, **1987**, 326, 347-52	50.4	640
289	Insights into DNA recombination from the structure of a RAD51-BRCA2 complex. *Nature*, **2002**, 420, 287-93	50.4	518
288	mCSM: predicting the effects of mutations in proteins using graph-based signatures. *Bioinformatics*, **2014**, 30, 335-42	7.2	505
287	Definition of general topological equivalence in protein structures. A procedure involving comparison of properties and relationships through simulated annealing and dynamic programming. *Journal of Molecular Biology*, **1990**, 212, 403-28	6.5	477
286	The molecular structure and stability of the eye lens: x-ray analysis of gamma-crystallin II. *Nature*, **1981**, 289, 771-7	50.4	460
285	New protein fold revealed by a 2.3-A resolution crystal structure of nerve growth factor. *Nature*, **1991**, 354, 411-4	50.4	453
284	DUET: a server for predicting effects of mutations on protein stability using an integrated computational approach. *Nucleic Acids Research*, **2014**, 42, W314-9	20.1	437
283	Structure of Rhombohedral 2 Zinc Insulin Crystals. *Nature*, **1969**, 224, 491-495	50.4	435
282	High-throughput crystallography for lead discovery in drug design. *Nature Reviews Drug Discovery*, **2002**, 1, 45-54	64.1	432
281	X-ray analysis of HIV-1 proteinase at 2.7 A resolution confirms structural homology among retroviral enzymes. *Nature*, **1989**, 342, 299-302	50.4	428
280	Structure of pentameric human serum amyloid P component. *Nature*, **1994**, 367, 338-45	50.4	422
279	HOMSTRAD: a database of protein structure alignments for homologous families. *Protein Science*, **1998**, 7, 2469-71	6.3	421

278	Structural evidence for gene duplication in the evolution of the acid proteases. *Nature*, **1978**, 271, 618-21	50.4	415
277	Receptor-binding region of insulin. *Nature*, **1976**, 259, 369-73	50.4	406
276	JOY: protein sequence-structure representation and analysis. *Bioinformatics*, **1998**, 14, 617-23	7.2	356
275	SDM--a server for predicting effects of mutations on protein stability and malfunction. *Nucleic Acids Research*, **2011**, 39, W215-22	20.1	343
274	Knowledge based modelling of homologous proteins, Part I: Three-dimensional frameworks derived from the simultaneous superposition of multiple structures. *Protein Engineering, Design and Selection*, **1987**, 1, 377-84	1.9	317
273	Atomic positions in rhombohedral 2-zinc insulin crystals. *Nature*, **1971**, 231, 506-11	50.4	297
272	X-ray analysis of glucagon and its relationship to receptor binding. *Nature*, **1975**, 257, 751-7	50.4	282
271	X-ray analysis (1. 4-A resolution) of avian pancreatic polypeptide: Small globular protein hormone. *Proceedings of the National Academy of Sciences of the United States of America*, **1981**, 78, 4175-9	11.5	271
270	Structural biology and drug discovery. *Drug Discovery Today*, **2005**, 10, 895-907	8.8	261
269	SDM: a server for predicting effects of mutations on protein stability. *Nucleic Acids Research*, **2017**, 45, W229-W235	20.1	246
268	Environment-specific amino acid substitution tables: tertiary templates and prediction of protein folds. *Protein Science*, **1992**, 1, 216-26	6.3	236
267	Insulin-like growth factor: a model for tertiary structure accounting for immunoreactivity and receptor binding. *Proceedings of the National Academy of Sciences of the United States of America*, **1978**, 75, 180-4	11.5	233
266	Solvent-induced distortions and the curvature of alpha-helices. *Nature*, **1983**, 306, 281-3	50.4	221
265	Structure-based drug design. *Nature*, **1996**, 384, 23-6	50.4	211
264	X-ray analyses of aspartic proteinases. II. Three-dimensional structure of the hexagonal crystal form of porcine pepsin at 2.3 A resolution. *Journal of Molecular Biology*, **1990**, 214, 199-222	6.5	211
263	18th Sir Hans Krebs lecture. Knowledge-based protein modelling and design. *FEBS Journal*, **1988**, 172, 513-20		211
262	The active site of aspartic proteinases. *FEBS Letters*, **1984**, 174, 96-101	3.8	211
261	DNA repair. PAXX, a paralog of XRCC4 and XLF, interacts with Ku to promote DNA double-strand break repair. *Science*, **2015**, 347, 185-188	33.3	202

260	Three-dimensional structure, specificity and catalytic mechanism of renin. *Nature*, **1983**, 304, 273-5	50.4	202
259	Crystal structure of an Xrcc4-DNA ligase IV complex. *Nature Structural Biology*, **2001**, 8, 1015-9		200
258	Arpeggio: A Web Server for Calculating and Visualising Interatomic Interactions in Protein Structures. *Journal of Molecular Biology*, **2017**, 429, 365-371	6.5	195
257	Knowledge based modelling of homologous proteins, Part II: Rules for the conformations of substituted sidechains. *Protein Engineering, Design and Selection*, **1987**, 1, 385-92	1.9	194
256	Crystal structure of the complex of the cyclin D-dependent kinase Cdk6 bound to the cell-cycle inhibitor p19INK4d. *Nature*, **1998**, 395, 244-50	50.4	187
255	Structure of porphobilinogen deaminase reveals a flexible multidomain polymerase with a single catalytic site. *Nature*, **1992**, 359, 33-9	50.4	187
254	Knowledge-based protein modeling. *Critical Reviews in Biochemistry and Molecular Biology*, **1994**, 29, 1-68	8.7	174
253	Structural biology in fragment-based drug design. *Current Opinion in Structural Biology*, **2010**, 20, 497-507	8.1	173
252	Conformational flexibility in a small globular hormone: x-ray analysis of avian pancreatic polypeptide at 0.98-A resolution. *Biopolymers*, **1983**, 22, 293-304	2.2	173
251	Tertiary structural constraints on protein evolutionary diversity: templates, key residues and structure prediction. *Proceedings of the Royal Society B: Biological Sciences*, **1990**, 241, 132-45	4.4	170
250	A three-dimensional model of the Photosystem II reaction centre of Pisum sativum. *Photosynthesis Research*, **1992**, 34, 287-300	3.7	167
249	Crystal structure of DNA-PKcs reveals a large open-ring cradle comprised of HEAT repeats. *Nature*, **2010**, 463, 118-21	50.4	165
248	Prediction of the stability of protein mutants based on structural environment-dependent amino acid substitution and propensity tables. *Protein Engineering, Design and Selection*, **1997**, 10, 7-21	1.9	162
247	Structural biology and drug discovery of difficult targets: the limits of ligandability. *Chemistry and Biology*, **2012**, 19, 42-50		159
246	Alignment and searching for common protein folds using a data bank of structural templates. *Journal of Molecular Biology*, **1993**, 231, 735-52	6.5	157
245	Functional map and domain structure of MET, the product of the c-met protooncogene and receptor for hepatocyte growth factor/scatter factor. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 12039-44	11.5	149
244	Molecular evolution and domain structure of plasminogen-related growth factors (HGF/SF and HGF1/MSP). *Protein Science*, **1994**, 3, 2378-94	6.3	146
243	Is the evolution of insulin Darwinian or due to selectively neutral mutation?. *Nature*, **1975**, 257, 197-203	50.4	143

242	X-ray analyses of peptide-inhibitor complexes define the structural basis of specificity for human and mouse renins. *Nature*, **1992**, 357, 466-72	50.4	141
241	Identification of the autophosphorylation sites and characterization of their effects in the protein kinase DYRK1A. *Biochemical Journal*, **2001**, 359, 497-505	3.8	133
240	Atomic interactions and profile of small molecules disrupting protein-protein interfaces: the TIMBAL database. *Chemical Biology and Drug Design*, **2009**, 74, 457-67	2.9	132
239	Structural biology and drug discovery for protein-protein interactions. *Trends in Pharmacological Sciences*, **2012**, 33, 241-8	13.2	130
238	High resolution X-ray analyses of renin inhibitor-aspartic proteinase complexes. *Nature*, **1987**, 327, 349-52	50.4	130
237	CODA: a combined algorithm for predicting the structurally variable regions of protein models. *Protein Science*, **2001**, 10, 599-612	6.3	129
236	Probing hot spots at protein-ligand binding sites: a fragment-based approach using biophysical methods. *Journal of Medicinal Chemistry*, **2006**, 49, 4992-5000	8.3	128
235	Modeling alpha-helical transmembrane domains: the calculation and use of substitution tables for lipid-facing residues. *Protein Science*, **1993**, 2, 55-70	6.3	127
234	Myxococcus xanthus spore coat protein S may have a similar structure to vertebrate lens beta gamma-crystallins. *Nature*, **1985**, 315, 771-3	50.4	123
233	Evolutionary trace analysis of TGF-beta and related growth factors: implications for site-directed mutagenesis. *Protein Engineering, Design and Selection*, **2000**, 13, 839-47	1.9	122
232	Application of fragment growing and fragment linking to the discovery of inhibitors of Mycobacterium tuberculosis pantothenate synthetase. *Angewandte Chemie - International Edition*, **2009**, 48, 8452-6	16.4	120
231	Structural biology and bioinformatics in drug design: opportunities and challenges for target identification and lead discovery. *Philosophical Transactions of the Royal Society B: Biological Sciences*, **2006**, 361, 413-23	5.8	115
230	Homology among acid proteases: comparison of crystal structures at 3A resolution of acid proteases from Rhizopus chinensis and Endothia parasitica. *Proceedings of the National Academy of Sciences of the United States of America*, **1977**, 74, 556-9	11.5	115
229	DNA-PKcs structure suggests an allosteric mechanism modulating DNA double-strand break repair. *Science*, **2017**, 355, 520-524	33.3	114
228	Three-dimensional atomic structure of insulin and its relationship to activity. *Diabetes*, **1972**, 21, 492-505	0.9	112
227	Eye-lens proteins: the three-dimensional structure of beta-crystallin predicted from monomeric gamma-crystallin. *FEBS Letters*, **1981**, 133, 9-16	3.8	104
226	Crystal structure of the pleckstrin homology domain from dynamin. *Nature Structural Biology*, **1994**, 1, 782-8		102
225	Direct observation by X-ray analysis of the tetrahedral "intermediate" of aspartic proteinases. *Protein Science*, **1992**, 1, 322-8	6.3	100

224	Using a fragment-based approach to target protein-protein interactions. *ChemBioChem*, **2013**, 14, 332-42	3.8	99
223	Molecular mechanism of SSR128129E, an extracellularly acting, small-molecule, allosteric inhibitor of FGF receptor signaling. *Cancer Cell*, **2013**, 23, 489-501	24.3	99
222	Crystal structure of the NK1 fragment of HGF/SF suggests a novel mode for growth factor dimerization and receptor binding. *Nature Structural Biology*, **1999**, 6, 72-9		99
221	Crystal structure of human XLF/Cernunnos reveals unexpected differences from XRCC4 with implications for NHEJ. *EMBO Journal*, **2008**, 27, 290-300	13	98
220	Domain flexibility in aspartic proteinases. *Proteins: Structure, Function and Bioinformatics*, **1992**, 12, 158-70	4.2	98
219	Computer graphics modelling of human renin. Specificity, catalytic activity and intron-exon junctions. *FEBS Letters*, **1984**, 174, 102-11	3.8	96
218	Conformational analysis and clustering of short and medium size loops connecting regular secondary structures: a database for modeling and prediction. *Protein Science*, **1996**, 5, 2600-16	6.3	94
217	Relaxin has conformational homology with insulin. *Nature*, **1977**, 270, 449-51	50.4	94
216	Crystal structures of NK1-heparin complexes reveal the basis for NK1 activity and enable engineering of potent agonists of the MET receptor. *EMBO Journal*, **2001**, 20, 5543-55	13	93
215	High-throughput X-ray crystallography for drug discovery. *Current Opinion in Pharmacology*, **2004**, 4, 490-6	5.1	91
214	Towards a resolution of the stoichiometry of the fibroblast growth factor (FGF)-FGF receptor-heparin complex. *Journal of Molecular Biology*, **2004**, 339, 821-34	6.5	91
213	Molecular anatomy: phyletic relationships derived from three-dimensional structures of proteins. *Journal of Molecular Evolution*, **1990**, 30, 43-59	3.1	91
212	Respiratory flexibility in response to inhibition of cytochrome C oxidase in Mycobacterium tuberculosis. *Antimicrobial Agents and Chemotherapy*, **2014**, 58, 6962-5	5.9	89
211	Flexibility and small pockets at protein-protein interfaces: New insights into druggability. *Progress in Biophysics and Molecular Biology*, **2015**, 119, 2-9	4.7	89
210	mCSM-lig: quantifying the effects of mutations on protein-small molecule affinity in genetic disease and emergence of drug resistance. *Scientific Reports*, **2016**, 6, 29575	4.9	88
209	Crystal structure of folliculin reveals a hidDENN function in genetically inherited renal cancer. *Open Biology*, **2012**, 2, 120071	7	84
208	Integrated biophysical approach to fragment screening and validation for fragment-based lead discovery. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 12984-9	11.5	83
207	Distinguishing structural and functional restraints in evolution in order to identify interaction sites. *Journal of Molecular Biology*, **2004**, 342, 1487-504	6.5	83

206	Catching a common fold. *Protein Science*, **1993**, 2, 877-83	6.3	83
205	Mutations at protein-protein interfaces: Small changes over big surfaces have large impacts on human health. *Progress in Biophysics and Molecular Biology*, **2017**, 128, 3-13	4.7	81
204	Symmetry, stability, and dynamics of multidomain and multicomponent protein systems. *Proceedings of the National Academy of Sciences of the United States of America*, **1996**, 93, 14243-8	11.5	80
203	Exploration of subsite binding specificity of human cathepsin D through kinetics and rule-based molecular modeling. *Protein Science*, **1993**, 2, 264-76	6.3	80
202	Biophysical and computational fragment-based approaches to targeting protein-protein interactions: applications in structure-guided drug discovery. *Quarterly Reviews of Biophysics*, **2012**, 45, 383-426	7	74
201	Comparative modelling of barley-grain aspartic proteinase: a structural rationale for observed hydrolytic specificity. *FEBS Letters*, **1994**, 352, 131-6	3.8	72
200	Twelve novel HGD gene variants identified in 99 alkaptonuria patients: focus on 'black bone disease' in Italy. *European Journal of Human Genetics*, **2016**, 24, 66-72	5.3	71
199	Evidence that heparin saccharides promote FGF2 mitogenesis through two distinct mechanisms. *Journal of Biological Chemistry*, **2008**, 283, 13001-8	5.4	71
198	The three-dimensional structures of mutants of porphobilinogen deaminase: toward an understanding of the structural basis of acute intermittent porphyria. *Protein Science*, **1994**, 3, 1644-50	6.3	70
197	The 3-D structure of HIV-1 proteinase and the design of antiviral agents for the treatment of AIDS. *Trends in Biochemical Sciences*, **1990**, 15, 425-30	10.3	70
196	In silico functional dissection of saturation mutagenesis: Interpreting the relationship between phenotypes and changes in protein stability, interactions and activity. *Scientific Reports*, **2016**, 6, 19848	4.9	68
195	An automatic method involving cluster analysis of secondary structures for the identification of domains in proteins. *Protein Science*, **1995**, 4, 506-20	6.3	66
194	X-ray structure of human stromelysin catalytic domain complexed with nonpeptide inhibitors: implications for inhibitor selectivity. *Protein Science*, **1999**, 8, 1455-62	6.3	66
193	Characterization and modelling of VanT: a novel, membrane-bound, serine racemase from vancomycin-resistant Enterococcus gallinarum BM4174. *Molecular Microbiology*, **1999**, 31, 1653-64	4.1	65
192	CREDO: a protein-ligand interaction database for drug discovery. *Chemical Biology and Drug Design*, **2009**, 73, 157-67	2.9	64
191	The crystal structure of E. coli pantothenate synthetase confirms it as a member of the cytidylyltransferase superfamily. *Structure*, **2001**, 9, 439-50	5.2	64
190	Identifying Interactions that Determine Fragment Binding at Protein Hotspots. *Journal of Medicinal Chemistry*, **2016**, 59, 4314-25	8.3	64
189	Cooperative dimerization of fibroblast growth factor 1 (FGF1) upon a single heparin saccharide may drive the formation of 2:2:1 FGF1.FGFR2c.heparin ternary complexes. *Journal of Biological Chemistry*, **2005**, 280, 42274-82	5.4	63

188	The Inosine Monophosphate Dehydrogenase, GuaB2, Is a Vulnerable New Bactericidal Drug Target for Tuberculosis. *ACS Infectious Diseases*, **2017**, 3, 5-17	5.5	62
187	Essential but Not Vulnerable: Indazole Sulfonamides Targeting Inosine Monophosphate Dehydrogenase as Potential Leads against Mycobacterium tuberculosis. *ACS Infectious Diseases*, **2017**, 3, 18-33	5.5	62
186	Germline Mutations in the CDKN2B Tumor Suppressor Gene Predispose to Renal Cell Carcinoma. *Cancer Discovery*, **2015**, 5, 723-9	24.4	61
185	Different DNA End Configurations Dictate Which NHEJ Components Are Most Important for Joining Efficiency. *Journal of Biological Chemistry*, **2016**, 291, 24377-24389	5.4	60
184	The structure of a synthetic pepsin inhibitor complexed with endothiapepsin. *FEBS Journal*, **1987**, 169, 215-21		60
183	Mutations in the NHEJ component XRCC4 cause primordial dwarfism. *American Journal of Human Genetics*, **2015**, 96, 412-24	11	59
182	Non-homologous end-joining partners in a helical dance: structural studies of XLF-XRCC4 interactions. *Biochemical Society Transactions*, **2011**, 39, 1387-92, suppl 2 p following 1392	5.1	59
181	Platinum: a database of experimentally measured effects of mutations on structurally defined protein-ligand complexes. *Nucleic Acids Research*, **2015**, 43, D387-91	20.1	58
180	Nerve growth factor: structure/function relationships. *Protein Science*, **1994**, 3, 1901-13	6.3	57
179	The spatial organization of non-homologous end joining: from bridging to end joining. *DNA Repair*, **2014**, 17, 98-109	4.3	55
178	Innate immunity. A Spaetzle-like role for nerve growth factor in vertebrate immunity to Staphylococcus aureus. *Science*, **2014**, 346, 641-646	33.3	55
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176	A novel exhaustive search algorithm for predicting the conformation of polypeptide segments in proteins. *Proteins: Structure, Function and Bioinformatics*, **2000**, 40, 135-144	4.2	53
175	Structural bioinformatics mutation analysis reveals genotype-phenotype correlations in von Hippel-Lindau disease and suggests molecular mechanisms of tumorigenesis. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 84-96	4.2	50
174	PDBe-KB: a community-driven resource for structural and functional annotations. *Nucleic Acids Research*, **2020**, 48, D344-D353	20.1	50
173	Dissection of DNA double-strand-break repair using novel single-molecule forceps. *Nature Structural and Molecular Biology*, **2018**, 25, 482-487	17.6	49
172	Protein crystallography and drug discovery: recollections of knowledge exchange between academia and industry. *IUCrJ*, **2017**, 4, 308-321	4.7	48
171	Structure of BRCA1-BRCT/Abraxas Complex Reveals Phosphorylation-Dependent BRCT Dimerization at DNA Damage Sites. *Molecular Cell*, **2016**, 61, 434-448	17.6	48

170	Genome3D: a UK collaborative project to annotate genomic sequences with predicted 3D structures based on SCOP and CATH domains. *Nucleic Acids Research*, **2013**, 41, D499-507	20.1	48
169	Andante: reducing side-chain rotamer search space during comparative modeling using environment-specific substitution probabilities. *Bioinformatics*, **2007**, 23, 1099-105	7.2	46
168	Protein-protein interactions in receptor activation and intracellular signalling. *Biological Chemistry*, **2000**, 381, 955-9	4.5	45
167	Structure of the catalytic region of DNA ligase IV in complex with an Artemis fragment sheds light on double-strand break repair. *Structure*, **2013**, 21, 672-9	5.2	44
166	Comprehensive, atomic-level characterization of structurally characterized protein-protein interactions: the PICCOLO database. *BMC Bioinformatics*, **2011**, 12, 313	3.6	44
165	Multimers of the fibroblast growth factor (FGF)-FGF receptor-saccharide complex are formed on long oligomers of heparin. *Biochemical Journal*, **2006**, 393, 741-8	3.8	44
164	BIPA: a database for protein-nucleic acid interaction in 3D structures. *Bioinformatics*, **2009**, 25, 1559-60	7.2	42
163	Arginine-deprivation-induced oxidative damage sterilizes. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 9779-9784	11.5	41
162	Cooperative heparin-mediated oligomerization of fibroblast growth factor-1 (FGF1) precedes recruitment of FGFR2 to ternary complexes. *Biophysical Journal*, **2013**, 104, 1720-30	2.9	40
161	The three-dimensional structure of Escherichia coli porphobilinogen deaminase at 1.76-A resolution. *Proteins: Structure, Function and Bioinformatics*, **1996**, 25, 48-78	4.2	38
160	Analysis of HGD Gene Mutations in Patients with Alkaptonuria from the United Kingdom: Identification of Novel Mutations. *JIMD Reports*, **2015**, 24, 3-11	1.9	36
159	Structural genomics: an overview. *Progress in Biophysics and Molecular Biology*, **2000**, 73, 289-95	4.7	35
158	X-ray crystallographic analysis of inhibition of endothiapepsin by cyclohexyl renin inhibitors. *Biochemistry*, **1992**, 31, 8142-50	3.2	35
157	Structural insights into the role of domain flexibility in human DNA ligase IV. *Structure*, **2012**, 20, 1212-22	5.2	34
156	Genome3D: exploiting structure to help users understand their sequences. *Nucleic Acids Research*, **2015**, 43, D382-6	20.1	33
155	Structural investigation of inhibitor designs targeting 3-dehydroquinate dehydratase from the shikimate pathway of Mycobacterium tuberculosis. *Biochemical Journal*, **2011**, 436, 729-39	3.8	33
154	Fragment-Based Approach to Targeting Inosine-5'-monophosphate Dehydrogenase (IMPDH) from Mycobacterium tuberculosis. *Journal of Medicinal Chemistry*, **2018**, 61, 2806-2822	8.3	32
153	A fragment merging approach towards the development of small molecule inhibitors of Mycobacterium tuberculosis EthR for use as ethionamide boosters. *Organic and Biomolecular Chemistry*, **2016**, 14, 2318-26	3.9	32

152	Small-molecule inhibitors that target protein-protein interactions in the RAD51 family of recombinases. *ChemMedChem*, **2015**, 10, 296-303	3.7	31
151	Characterization of symmetric complexes of nerve growth factor and the ectodomain of the pan-neurotrophin receptor, p75NTR. *Journal of Biological Chemistry*, **2005**, 280, 33453-60	5.4	31
150	CREDO: a structural interactomics database for drug discovery. *Database: the Journal of Biological Databases and Curation*, **2013**, 2013, bat049	5	30
149	Dimers of DNA-PK create a stage for DNA double-strand break repair. *Nature Structural and Molecular Biology*, **2021**, 28, 13-19	17.6	30
148	Targeting tuberculosis using structure-guided fragment-based drug design. *Drug Discovery Today*, **2017**, 22, 546-554	8.8	29
147	An iterative structure-assisted approach to sequence alignment and comparative modeling **1999**, 37, 55-60		29
146	Structural and functional restraints on the occurrence of single amino acid variations in human proteins. *PLoS ONE*, **2010**, 5, e9186	3.7	29
145	Structural Implications of Mutations Conferring Rifampin Resistance in Mycobacterium leprae. *Scientific Reports*, **2018**, 8, 5016	4.9	28
144	A structure-guided fragment-based approach for the discovery of allosteric inhibitors targeting the lipophilic binding site of transcription factor EthR. *Biochemical Journal*, **2014**, 458, 387-94	3.8	27
143	Exploring the binding preferences/specificity in the active site of human cathepsin E. *Proteins: Structure, Function and Bioinformatics*, **1995**, 22, 168-81	4.2	27
142	Genomes, structural biology and drug discovery: combating the impacts of mutations in genetic disease and antibiotic resistance. *Biochemical Society Transactions*, **2017**, 45, 303-311	5.1	26
141	Structural Biology and the Design of New Therapeutics: From HIV and Cancer to Mycobacterial Infections: A Paper Dedicated to John Kendrew. *Journal of Molecular Biology*, **2017**, 429, 2677-2693	6.5	26
140	Insights into the structure of hepatocyte growth factor/scatter factor (HGF/SF) and implications for receptor activation. *FEBS Letters*, **1998**, 430, 126-9	3.8	26
139	Structural analysis of DNA-PKcs: modelling of the repeat units and insights into the detailed molecular architecture. *Journal of Structural Biology*, **2004**, 145, 295-306	3.4	25
138	Decoding the similarities and differences among mycobacterial species. *PLoS Neglected Tropical Diseases*, **2017**, 11, e0005883	4.8	24
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136	Phosphopeptide interactions with BRCA1 BRCT domains: More than just a motif. *Progress in Biophysics and Molecular Biology*, **2015**, 117, 143-148	4.7	23
135	Exploring the chemical space of the lysine-binding pocket of the first kringle domain of hepatocyte growth factor/scatter factor (HGF/SF) yields a new class of inhibitors of HGF/SF-MET binding. *Chemical Science*, **2015**, 6, 6147-6157	9.4	23

134	Lst4, the yeast Fnip1/2 orthologue, is a DENN-family protein. *Open Biology*, **2015**, 5, 150174	7	23
133	Structural biology of DNA repair: spatial organisation of the multicomponent complexes of nonhomologous end joining. *Journal of Nucleic Acids*, **2010**, 2010,	2.3	23
132	Structural aspects of the functional modules in human protein kinase-C alpha deduced from comparative analyses. *Proteins: Structure, Function and Bioinformatics*, **1996**, 26, 217-35	4.2	23
131	Stepwise pathogenic evolution of. *Science*, **2021**, 372,	33.3	23
130	Spatial and temporal organization of multi-protein assemblies: achieving sensitive control in information-rich cell-regulatory systems. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2012**, 370, 3023-39	3	22
129	Cleavage efficiency of the novel aspartic protease yapsin 1 (Yap3p) enhanced for substrates with arginine residues flanking the P1 site: correlation with electronegative active-site pockets predicted by molecular modeling. *Biochemistry*, **1998**, 37, 2768-77	3.2	22
128	Prediction of impacts of mutations on protein structure and interactions: SDM, a statistical approach, and mCSM, using machine learning. *Protein Science*, **2020**, 29, 247-257	6.3	22
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126	Incorporating knowledge-based biases into an energy-based side-chain modeling method: application to comparative modeling of protein structure. *Biopolymers*, **2001**, 59, 72-86	2.2	21
125	Mechanism of efficient double-strand break repair by a long non-coding RNA. *Nucleic Acids Research*, **2020**, 48, 10953-10972	20.1	21
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118	CHOPIN: a web resource for the structural and functional proteome of Mycobacterium tuberculosis. *Database: the Journal of Biological Databases and Curation*, **2015**, 2015,	5	19
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