Tom Blundell

List of Publications by Year
in descending order

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315 papers	44,143 citations	3726 89 h-index	2178 202 g-index
334 all docs	334 docs citations	334 times ranked	43084 citing authors

#	Article	IF	Citations
1	Comparative Protein Modelling by Satisfaction of Spatial Restraints. Journal of Molecular Biology, 1993, 234, 779-815.	2.0	11,892
2	pkCSM: Predicting Small-Molecule Pharmacokinetic and Toxicity Properties Using Graph-Based Signatures. Journal of Medicinal Chemistry, 2015, 58, 4066-4072.	2.9	2,335
3	FUGUE: sequence-structure homology recognition using environment-specific substitution tables and structure-dependent gap penalties11Edited by B. Honig. Journal of Molecular Biology, 2001, 310, 243-257.	2.0	1,185
4	The TRANSPARENT TESTA GLABRA1 Locus, Which Regulates Trichome Differentiation and Anthocyanin Biosynthesis in Arabidopsis, Encodes a WD40 Repeat Protein. Plant Cell, 1999, 11, 1337-1349.	3.1	905
5	mCSM: predicting the effects of mutations in proteins using graph-based signatures. Bioinformatics, 2014, 30, 335-342.	1.8	779
6	Crystal structure of fibroblast growth factor receptor ectodomain bound to ligand and heparin. Nature, 2000, 407, 1029-1034.	13.7	704
7	Knowledge-based prediction of protein structures and the design of novel molecules. Nature, 1987, 326, 347-352.	13.7	692
8	DUET: a server for predicting effects of mutations on protein stability using an integrated computational approach. Nucleic Acids Research, 2014, 42, W314-W319.	6.5	664
9	Insights into DNA recombination from the structure of a RAD51â€“BRCA2 complex. Nature, 2002, 420, 287-293.	13.7	615
10	Structure of Rhombohedral 2 Zinc Insulin Crystals. Nature, 1969, 224, 491-495.	13.7	532
11	Definition of general topological equivalence in protein structures. Journal of Molecular Biology, 1990, 212, 403-428.	2.0	509
12	New protein fold revealed by a 2.3-Ã... resolution crystal structure of nerve growth factor. Nature, 1991, 354, 411-414.	13.7	500
13	High-throughput crystallography for lead discovery in drug design. Nature Reviews Drug Discovery, 2002, 1, 45-54.	21.5	490
14	The molecular structure and stability of the eye lens: X-ray analysis of Î³-crystallin II. Nature, 1981, 289, 771-777.	13.7	480
15	X-ray analysis of HIV-1 proteinase at 2.7 Ã... resolution confirms structural homology among retroviral enzymes. Nature, 1989, 342, 299-302.	13.7	477
16	Structure of pentameric human serum amyloid P component. Nature, 1994, 367, 338-345.	13.7	471
17	HOMSTRAD: A database of protein structure alignments for homologous families. Protein Science, 1998, 7, 2469-2471.	3.1	461
18	SDM--a server for predicting effects of mutations on protein stability and malfunction. Nucleic Acids Research, 2011, 39, W215-W222.	6.5	453

#	Article	IF	Citations
19	Receptor-binding region of insulin. Nature, 1976, 259, 369-373.	13.7	444
20	Structural evidence for gene duplication in the evolution of the acid proteases. Nature, 1978, 271, 618-621.	13.7	441
21	SDM: a server for predicting effects of mutations on protein stability. Nucleic Acids Research, 2017, 45, W229-W235.	6.5	407
22	JOY: protein sequence-structure representation and analysis. Bioinformatics, 1998, 14, 617-623.	1.8	384
23	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, 377-384.	1.0	365
24	Arpeggio: A Web Server for Calculating and Visualising Interatomic Interactions in Protein Structures. Journal of Molecular Biology, 2017, 429, 365-371.	2.0	340
25	Atomic Positions in Rhombohedral 2-Zinc Insulin Crystals. Nature, 1971, 231, 506-511.	13.7	328
26	Keynote review: Structural biology and drug discovery. Drug Discovery Today, 2005, 10, 895-907.	3.2	311
27	X-ray analysis of glucagon and its relationship to receptor binding. Nature, 1975, 257, 751-757.	13.7	305
28	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, 4175-4179.	3.3	298
29	Environmentâ€specific amino acid substitution tables: Tertiary templates and prediction of protein folds. Protein Science, 1992, 1, 216-226.	3.1	288
30	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, 180-184.	3.3	258
31	PAXX, a paralog of XRCC4 and XLF, interacts with Ku to promote DNA double-strand break repair. Science, 2015, 347, 185-188.	6.0	252
32	The active site of aspartic proteinases. FEBS Letters, 1984, 174, 96-101.	1.3	242
33	Knowledge-based protein modelling and design. FEBS Journal, 1988, 172, 513-520.	0.2	236
34	Signalling the fat controller. Nature, 1996, 384, 23-24.	13.7	236
35	Solvent-induced distortions and the curvature of Î±-helices. Nature, 1983, 306, 281-283.	13.7	235
36	Three-dimensional structure, specificity and catalytic mechanism of renin. Nature, 1983, 304, 273-275.	13.7	229

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37	Crystal structure of an Xrcc4-DNA ligase IV complex. Nature Structural Biology, 2001, 8, 1015-1019.	9.7	229
38	X-ray analyses of aspartic proteinases. Journal of Molecular Biology, 1990, 214, 199-222.	2.0	224
39	Knowledge based modelling of homologous proteins, part II: rules for the conformations of substituted sidechains. Protein Engineering, Design and Selection, 1987, 1, 385-392.	1.0	222
40	Structure of porphobilinogen deaminase reveals a flexible multidomain polymerase with a single catalytic site. Nature, 1992, 359, 33-39.	13.7	213
41	Knowledge-Based Protein Modeling. Critical Reviews in Biochemistry and Molecular Biology, 1994, 29, 1-68.	2.3	206
42	Conformational flexibility in a small globular hormone: X-ray analysis of avian pancreatic polypeptide at 0.98-Ã... resolution. Biopolymers, 1983, 22, 293-304.	1.2	204
43	Tertiary structural constraints on protein evolutionary diversity: templates, key residues and structure prediction. Proceedings of the Royal Society B: Biological Sciences, 1990, 241, 132-145.	1.2	203
44	Crystal structure of the complex of the cyclin D-dependent kinase Cdk6 bound to the cell-cycle inhibitor p19INK4d. Nature, 1998, 395, 244-250.	13.7	199
45	Crystal structure of DNA-PKcs reveals a large open-ring cradle comprised of HEAT repeats. Nature, 2010, 463, 118-121.	13.7	195
46	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.	1.0	191
47	Structural Biology and Drug Discovery of Difficult Targets: The Limits of Ligandability. Chemistry and Biology, 2012, 19, 42-50.	6.2	191
48	Structural biology in fragment-based drug design. Current Opinion in Structural Biology, 2010, 20, 497-507.	2.6	190
49	Alignment and Searching for Common Protein Folds Using a Data Bank of Structural Templates. Journal of Molecular Biology, 1993, 231, 735-752.	2.0	174
50	A three-dimensional model of the Photosystem II reaction centre of Pisum sativum. Photosynthesis Research, 1992, 34, 287-300.	1.6	170
51	Molecular evolution and domain structure of plasminogenâ€related growth factors (HGF/SF and) Tj ETQq1 1 0.784314 rgBT /Overlock	3.1	166
52	X-ray analyses of peptideâ€“inhibitor complexes define the structural basis of specificity for human and mouse renins. Nature, 1992, 357, 466-472.	13.7	163
53	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, 12039-12044.	3.3	163
54	Is the evolution of insulin Darwinian or due to selectively neutral mutation?. Nature, 1975, 257, 197-203.	13.7	161

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55	Identification of the autophosphorylation sites and characterization of their effects in the protein kinase DYRK1A. Biochemical Journal, 2001, 359, 497-505.	1.7	158
56	Structural biology and drug discovery for proteinâ€“protein interactions. Trends in Pharmacological Sciences, 2012, 33, 241-248.	4.0	155
57	DNA-PKcs structure suggests an allosteric mechanism modulating DNA double-strand break repair. Science, 2017, 355, 520-524.	6.0	155
58	CODA: A combined algorithm for predicting the structurally variable regions of protein models. Protein Science, 2001, 10, 599-612.	3.1	147
59	Atomic Interactions and Profile of Small Molecules Disrupting Proteinâ€“Protein Interfaces: the TIMBAL Database. Chemical Biology and Drug Design, 2009, 74, 457-467.	1.5	144
60	High resolution X-ray analyses of renin inhibitor-aspartic proteinase complexes. Nature, 1987, 327, 349-352.	13.7	143
61	Modeling Î±â€helical transmembrane domains: The calculation and use of substitution tables for lipidâ€facing residues. Protein Science, 1993, 2, 55-70.	3.1	143
62	Probing Hot Spots at Proteinâ^'Ligand Binding Sites:â€‰ A Fragment-Based Approach Using Biophysical Methods. Journal of Medicinal Chemistry, 2006, 49, 4992-5000.	2.9	140
63	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, 413-423.	1.8	140
64	Application of Fragment Growing and Fragment Linking to the Discovery of Inhibitors of Mycobacterium tuberculosis Pantothenate Synthetase. Angewandte Chemie - International Edition, 2009, 48, 8452-8456.	7.2	138
65	Myxococcus xanthus spore coat protein S may have a similar structure to vertebrate lens Î²Î³-crystallins. Nature, 1985, 315, 771-773.	13.7	134
66	Evolutionary trace analysis of TGF-Î² and related growth factors: implications for site-directed mutagenesis. Protein Engineering, Design and Selection, 2000, 13, 839-847.	1.0	130
67	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.	1.4	129
68	Molecular Mechanism of SSR128129E, an Extracellularly Acting, Small-Molecule, Allosteric Inhibitor of FGF Receptor Signaling. Cancer Cell, 2013, 23, 489-501.	7.7	125
69	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, 556-559.	3.3	123
70	Three-Dimensional Atomic Structure of Insulin and Its Relationship to Activity. Diabetes, 1972, 21, 492-505.	0.3	122
71	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.	1.6	120
72	Flexibility and small pockets at proteinâ€“protein interfaces: New insights into druggability. Progress in Biophysics and Molecular Biology, 2015, 119, 2-9.	1.4	118

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73	Respiratory Flexibility in Response to Inhibition of Cytochrome c Oxidase in Mycobacterium tuberculosis. Antimicrobial Agents and Chemotherapy, 2014, 58, 6962-6965.	1.4	116
74	Crystal structure of the pleckstrin homology domain from dynamin. Nature Structural Biology, 1994, 1, 782-788.	9.7	115
75	Using a Fragmentâ€Based Approach To Target Proteinâ€“Protein Interactions. ChemBioChem, 2013, 14, 332-342.	1.3	115
76	Eye-lens proteins: The three-dimensional structure of Î²-crystallin predicted from monomeric Î³-crystallin. FEBS Letters, 1981, 133, 9-16.	1.3	110
77	Computer graphics modelling of human renin. FEBS Letters, 1984, 174, 102-111.	1.3	110
78	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, 72-79.	9.7	110
79	Direct observation by Xâ€ray analysis of the tetrahedral â€œintermediateâ€•of aspartic proteinases. Protein Science, 1992, 1, 322-328.	3.1	107
80	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, 5543-5555.	3.5	107
81	Towards a Resolution of the Stoichiometry of the Fibroblast Growth Factor (FGF)â€“FGF Receptorâ€“Heparin Complex. Journal of Molecular Biology, 2004, 339, 821-834.	2.0	107
82	Domain flexibility in aspartic proteinases. Proteins: Structure, Function and Bioinformatics, 1992, 12, 158-170.	1.5	106
83	High-throughput X-ray crystallography for drug discovery. Current Opinion in Pharmacology, 2004, 4, 490-496.	1.7	106
84	Crystal structure of human XLF/Cernunnos reveals unexpected differences from XRCC4 with implications for NHEJ. EMBO Journal, 2008, 27, 290-300.	3.5	106
85	Molecular anatomy: Phyletic relationships derived from three-dimensional structures of proteins. Journal of Molecular Evolution, 1990, 30, 43-59.	0.8	103
86	Conformational analysis and clustering of short and medium size loops connecting regular secondary structures: A database for modeling and prediction. Protein Science, 1996, 5, 2600-2616.	3.1	103
87	Relaxin has conformational homology with insulin. Nature, 1977, 270, 449-451.	13.7	102
88	Crystal structure of folliculin reveals a hidDENN function in genetically inherited renal cancer. Open Biology, 2012, 2, 120071.	1.5	97
89	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, 12984-12989.	3.3	97
90	Arginine-deprivationâ€“induced oxidative damage sterilizes Mycobacterium tuberculosis. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 9779-9784.	3.3	97

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91	Catching a common fold. Protein Science, 1993, 2, 877-883.	3.1	95
92	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, 14243-14248.	3.3	93
93	Exploration of subsite binding specificity of human cathepsin D through kinetics and ruleâ€based molecular modeling. Protein Science, 1993, 2, 264-276.	3.1	91
94	Stepwise pathogenic evolution of Mycobacterium abscessus. Science, 2021, 372, .	6.0	91
95	Biophysical and computational fragment-based approaches to targeting proteinâ€“protein interactions: applications in structure-guided drug discovery. Quarterly Reviews of Biophysics, 2012, 45, 383-426.	2.4	90
96	Utilizing graph machine learning within drug discovery and development. Briefings in Bioinformatics, 2021, 22, .	3.2	90
97	Distinguishing Structural and Functional Restraints in Evolution in Order to Identify Interaction Sites. Journal of Molecular Biology, 2004, 342, 1487-1504.	2.0	89
98	Germline Mutations in the CDKN2B Tumor Suppressor Gene Predispose to Renal Cell Carcinoma. Cancer Discovery, 2015, 5, 723-729.	7.7	88
99	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.	1.6	87
100	Twelve novel HGD gene variants identified in 99 alkaptonuria patients: focus on â€˜black bone diseaseâ€™ in Italy. European Journal of Human Genetics, 2016, 24, 66-72.	1.4	87
101	PDBe-KB: a community-driven resource for structural and functional annotations. Nucleic Acids Research, 2020, 48, D344-D353.	6.5	87
102	Identifying Interactions that Determine Fragment Binding at Protein Hotspots. Journal of Medicinal Chemistry, 2016, 59, 4314-4325.	2.9	86
103	CREDO: A Proteinâ€“Ligand Interaction Database for Drug Discovery. Chemical Biology and Drug Design, 2009, 73, 157-167.	1.5	84
104	Different DNA End Configurations Dictate Which NHEJ Components Are Most Important for Joining Efficiency. Journal of Biological Chemistry, 2016, 291, 24377-24389.	1.6	83
105	The Inosine Monophosphate Dehydrogenase, GuaB2, Is a Vulnerable New Bactericidal Drug Target for Tuberculosis. ACS Infectious Diseases, 2017, 3, 5-17.	1.8	83
106	An automatic method involving cluster analysis of secondary structures for the identification of domains in proteins. Protein Science, 1995, 4, 506-520.	3.1	81
107	Platinum: a database of experimentally measured effects of mutations on structurally defined proteinâ€“ligand complexes. Nucleic Acids Research, 2015, 43, D387-D391.	6.5	81
108	Comparative modelling of barley-grain aspartic proteinase: A structural rationale for observed hydrolytic specificity. FEBS Letters, 1994, 352, 131-136.	1.3	80

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109	Dissection of DNA double-strand-break repair using novel single-molecule forceps. Nature Structural and Molecular Biology, 2018, 25, 482-487.	3.6	79
110	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, 425-430.	3.7	78
111	The threeâ€dimensional structures of mutants of porphobilinogen deaminase: Toward an understanding of the structural basis of acute intermittent porphyria. Protein Science, 1994, 3, 1644-1650.	3.1	77
112	Essential but Not Vulnerable: Indazole Sulfonamides Targeting Inosine Monophosphate Dehydrogenase as Potential Leads against Mycobacterium tuberculosis. ACS Infectious Diseases, 2017, 3, 18-33.	1.8	77
113	Evidence That Heparin Saccharides Promote FGF2 Mitogenesis through Two Distinct Mechanisms. Journal of Biological Chemistry, 2008, 283, 13001-13008.	1.6	76
114	Characterization and modelling of VanT: a novel, membrane-bound, serine racemase from vancomycin-resistant Enterococcus gallinarum BM4174. Molecular Microbiology, 1999, 31, 1653-1664.	1.2	75
115	Xâ€ray structure of human stromelysin catalytic domain complexed with nonpeptide inhibitors: Implications for inhibitor selectivity. Protein Science, 1999, 8, 1455-1462.	3.1	71
116	Mutations in the NHEJ Component XRCC4 Cause Primordial Dwarfism. American Journal of Human Genetics, 2015, 96, 412-424.	2.6	71
117	The Crystal Structure of E. coli Pantothenate Synthetase Confirms It as a Member of the Cytidylyltransferase Superfamily. Structure, 2001, 9, 439-450.	1.6	70
118	Nerve growth factor: Structure/function relationships. Protein Science, 1994, 3, 1901-1913.	3.1	69
119	Structure of mouse 7S NGF: a complex of nerve growth factor with four binding proteins. Structure, 1997, 5, 1275-1285.	1.6	68
120	Cooperative Dimerization of Fibroblast Growth Factor 1 (FGF1) upon a Single Heparin Saccharide May Drive the Formation of 2:2:1 FGF1Â·FGFR2cÂ·Heparin Ternary Complexes. Journal of Biological Chemistry, 2005, 280, 42274-42282.	1.6	68
121	A Spaetzle-like role for nerve growth factor Î² in vertebrate immunity to Staphylococcus aureus. Science, 2014, 346, 641-646.	6.0	68
122	Dimers of DNA-PK create a stage for DNA double-strand break repair. Nature Structural and Molecular Biology, 2021, 28, 13-19.	3.6	67
123	The structure of a synthetic pepsin inhibitor complexed with endothiapepsin. FEBS Journal, 1987, 169, 215-221.	0.2	66
124	Non-homologous end-joining partners in a helical dance: structural studies of XLFâ€“XRCC4 interactions. Biochemical Society Transactions, 2011, 39, 1387-1392.	1.6	65
125	Protein crystallography and drug discovery: recollections of knowledge exchange between academia and industry. IUCrJ, 2017, 4, 308-321.	1.0	65
126	Cryo-EM of NHEJ supercomplexes provides insights into DNA repair. Molecular Cell, 2021, 81, 3400-3409.e3.	4.5	62

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127	Structure of BRCA1-BRCT/Abraxas Complex Reveals Phosphorylation-Dependent BRCT Dimerization at DNA Damage Sites. Molecular Cell, 2016, 61, 434-448.	4.5	61
128	A novel exhaustive search algorithm for predicting the conformation of polypeptide segments in proteins. Proteins: Structure, Function and Bioinformatics, 2000, 40, 135-144.	1.5	60
129	The spatial organization of non-homologous end joining: From bridging to end joining. DNA Repair, 2014, 17, 98-109.	1.3	60
130	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.	3.1	58
131	Structural bioinformatics mutation analysis reveals genotypeâ€“phenotype correlations in von Hippelâ€Lindau disease and suggests molecular mechanisms of tumorigenesis. Proteins: Structure, Function and Bioinformatics, 2009, 77, 84-96.	1.5	57
132	Metalloproteinase superâ€“families and drug design. Nature Structural and Molecular Biology, 1994, 1, 73-75.	3.6	56
133	Comprehensive, atomic-level characterization of structurally characterized protein-protein interactions: the PICCOLO database. BMC Bioinformatics, 2011, 12, 313.	1.2	56
134	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, 672-679.	1.6	55
135	A second front against AIDS. Nature, 1989, 337, 596-597.	13.7	53
136	Genome3D: a UK collaborative project to annotate genomic sequences with predicted 3D structures based on SCOP and CATH domains. Nucleic Acids Research, 2012, 41, D499-D507.	6.5	53
137	Protein-Protein Interactions in Receptor Activation and Intracellular Signalling. Biological Chemistry, 2000, 381, 955-9.	1.2	51
138	Fragment-Based Approach to Targeting Inosine-5â€²-monophosphate Dehydrogenase (IMPDH) from Mycobacterium tuberculosis. Journal of Medicinal Chemistry, 2018, 61, 2806-2822.	2.9	51
139	BIPA: a database for proteinâ€“nucleic acid interaction in 3D structures. Bioinformatics, 2009, 25, 1559-1560.	1.8	50
140	Multimers of the fibroblast growth factor (FGF)â€“FGF receptorâ€“saccharide complex are formed on long oligomers of heparin. Biochemical Journal, 2006, 393, 741-748.	1.7	48
141	Andante: reducing side-chain rotamer search space during comparative modeling using environment-specific substitution probabilities. Bioinformatics, 2007, 23, 1099-1105.	1.8	48
142	PDBe-KB: collaboratively defining the biological context of structural data. Nucleic Acids Research, 2022, 50, D534-D542.	6.5	46
143	Structural Insights into the Role of Domain Flexibility in Human DNA Ligase IV. Structure, 2012, 20, 1212-1222.	1.6	44
144	Mechanism of efficient double-strand break repair by a long non-coding RNA. Nucleic Acids Research, 2020, 48, 10953-10972.	6.5	43

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145	Structural genomics: an overview. Progress in Biophysics and Molecular Biology, 2000, 73, 289-295.	1.4	42
146	Cooperative Heparin-Mediated Oligomerization of Fibroblast Growth Factor-1 (FGF1) Precedes Recruitment of FGFR2 to Ternary Complexes. Biophysical Journal, 2013, 104, 1720-1730.	0.2	42
147	Analysis of HGD Gene Mutations in Patients with Alkaptonuria from the United Kingdom: Identification of Novel Mutations. JIMD Reports, 2014, 24, 3-11.	0.7	42
148	Genome3D: exploiting structure to help users understand their sequences. Nucleic Acids Research, 2015, 43, D382-D386.	6.5	42
149	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, 2318-2326.	1.5	41
150	Structural Implications of Mutations Conferring Rifampin Resistance in Mycobacterium leprae. Scientific Reports, 2018, 8, 5016.	1.6	41
151	The three-dimensional structure ofEscherichia coliporphobilinogen deaminase at 1.76-Ã... resolution. , 1996, 25, 48-78.		40
152	Whole Exome Sequencing reveals NOTCH1 mutations in anaplastic large cell lymphoma and points to Notch both as a key pathway and a potential therapeutic target. Haematologica, 2021, 106, 1693-1704.	1.7	40
153	Structural investigation of inhibitor designs targeting 3-dehydroquinate dehydratase from the shikimate pathway of Mycobacterium tuberculosis. Biochemical Journal, 2011, 436, 729-739.	1.7	39
154	Structural Biology and the Design of New Therapeutics: From HIV and Cancer to Mycobacterial Infections. Journal of Molecular Biology, 2017, 429, 2677-2693.	2.0	39
155	Structural and Functional Restraints on the Occurrence of Single Amino Acid Variations in Human Proteins. PLoS ONE, 2010, 5, e9186.	1.1	38
156	X-ray crystallographic analysis of inhibition of endothiapepsin by cyclohexyl renin inhibitors. Biochemistry, 1992, 31, 8142-8150.	1.2	37
157	Decoding the similarities and differences among mycobacterial species. PLoS Neglected Tropical Diseases, 2017, 11, e0005883.	1.3	37
158	Systematic Investigation of the Data Set Dependency of Protein Stability Predictors. Journal of Chemical Information and Modeling, 2020, 60, 4772-4784.	2.5	37
159	Smallâ€Molecule Inhibitors That Target Proteinâ€“Protein Interactions in the RAD51 Family of Recombinases. ChemMedChem, 2015, 10, 296-303.	1.6	36
160	Targeting tuberculosis using structure-guided fragment-based drug design. Drug Discovery Today, 2017, 22, 546-554.	3.2	36
161	Structural insights into inhibitor regulation of the DNA repair protein DNA-PKcs. Nature, 2022, 601, 643-648.	13.7	36
162	CREDO: a structural interactomics database for drug discovery. Database: the Journal of Biological Databases and Curation, 2013, 2013, bat049.	1.4	35

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163	Genomes, structural biology and drug discovery: combating the impacts of mutations in genetic disease and antibiotic resistance. Biochemical Society Transactions, 2017, 45, 303-311.	1.6	35
164	Characterization of Symmetric Complexes of Nerve Growth Factor and the Ectodomain of the Pan-neurotrophin Receptor, p75NTR. Journal of Biological Chemistry, 2005, 280, 33453-33460.	1.6	34
165	Phosphopeptide interactions with BRCA1 BRCT domains: More than just a motif. Progress in Biophysics and Molecular Biology, 2015, 117, 143-148.	1.4	33
166	Identification of new allosteric sites and modulators of AChE through computational and experimental tools. Journal of Enzyme Inhibition and Medicinal Chemistry, 2018, 33, 1034-1047.	2.5	33
167	Exploring the binding preferences/specificity in the active site of human cathepsin E. Proteins: Structure, Function and Bioinformatics, 1995, 22, 168-181.	1.5	32
168	An iterative structure-assisted approach to sequence alignment and comparative modeling. , 1999, 37, 55-60.		32
169	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, 387-394.	1.7	32
170	Identification and Characterization of Genetic Determinants of Isoniazid and Rifampicin Resistance in Mycobacterium tuberculosis in Southern India. Scientific Reports, 2019, 9, 10283.	1.6	32
171	Development of Inhibitors against Mycobacterium abscessus tRNA (m¹G37) Methyltransferase (TrmD) Using Fragment-Based Approaches. Journal of Medicinal Chemistry, 2019, 62, 7210-7232.	2.9	32
172	SARS-CoV-2 3D database: understanding the coronavirus proteome and evaluating possible drug targets. Briefings in Bioinformatics, 2021, 22, 769-780.	3.2	31
173	Mycobacterium tuberculosis Dihydrofolate Reductase Reveals Two Conformational States and a Possible Low Affinity Mechanism to Antifolate Drugs. Structure, 2014, 22, 94-103.	1.6	30
174	Structure-guided fragment-based drug discovery at the synchrotron: screening binding sites and correlations with hotspot mapping. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180422.	1.6	30
175	Structural aspects of the functional modules in human protein kinase-CÎ± deduced from comparative analyses. , 1996, 26, 217-235.		29
176	Insights into the structure of hepatocyte growth factor/scatter factor (HGF/SF) and implications for receptor activation. FEBS Letters, 1998, 430, 126-129.	1.3	29
177	The deubiquitylating enzyme UCHL3 regulates Ku80 retention at sites of DNA damage. Scientific Reports, 2018, 8, 17891.	1.6	29
178	A third fibronectin type III domain in the extracellular region of the insulin receptor family. FEBS Letters, 1998, 441, 331-336.	1.3	28
179	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, 3023-3039.	1.6	28
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