Charlotte M Deane

List of Publications by Citations

197 papers	6,142 citations	40 h-index	71 g-index
290 ext. papers	8,017 ext. citations	6 avg, IF	6.4 L-index

#	Paper	IF	Citations
197	Protein interactions: two methods for assessment of the reliability of high throughput observations. *Molecular and Cellular Proteomics*, **2002**, 1, 349-56	7.6	486
196	HOMSTRAD: a database of protein structure alignments for homologous families. *Protein Science*, **1998**, 7, 2469-71	6.3	421
195	Reduced amounts and abnormal forms of phospholipase C zeta (PLCzeta) in spermatozoa from infertile men. *Human Reproduction*, **2009**, 24, 2417-28	5.7	208
194	SAbDab: the structural antibody database. *Nucleic Acids Research*, **2014**, 42, D1140-6	20.1	193
193	CODA: a combined algorithm for predicting the structurally variable regions of protein models. *Protein Science*, **2001**, 10, 599-612	6.3	129
192	Freely available conformer generation methods: how good are they?. *Journal of Chemical Information and Modeling*, **2012**, 52, 1146-58	6.1	128
191	FREAD revisited: Accurate loop structure prediction using a database search algorithm. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1431-40	4.2	128
190	Synonymous codon usage influences the local protein structure observed. *Nucleic Acids Research*, **2010**, 38, 6719-28	20.1	116
189	A multi-crystal method for extracting obscured crystallographic states from conventionally uninterpretable electron density. *Nature Communications*, **2017**, 8, 15123	17.4	115
188	Five computational developability guidelines for therapeutic antibody profiling. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 4025-4030	11.5	109
187	CoV-AbDab: the coronavirus antibody database. *Bioinformatics*, **2021**, 37, 734-735	7.2	108
186	ABodyBuilder: Automated antibody structure prediction with data-driven accuracy estimation. *MAbs*, **2016**, 8, 1259-1268	6.6	104
185	Revisiting date and party hubs: novel approaches to role assignment in protein interaction networks. *PLoS Computational Biology*, **2010**, 6, e1000817	5	100
184	ANARCI: antigen receptor numbering and receptor classification. *Bioinformatics*, **2016**, 32, 298-300	7.2	98
183	A maternally inherited autosomal point mutation in human phospholipase C zeta (PLC) leads to male infertility. *Human Reproduction*, **2012**, 27, 222-31	5.7	96
182	Avoiding False Positive Conclusions in Molecular Simulation: The Importance of Replicas. *Journal of Chemical Theory and Computation*, **2018**, 14, 6127-6138	6.4	94
181	MEDELLER: homology-based coordinate generation for membrane proteins. *Bioinformatics*, **2010**, 26, 2833-40	7.2	91

180	A microtubule interactome: complexes with roles in cell cycle and mitosis. *PLoS Biology*, **2008**, 6, e98	9.7	90
179	Improving B-cell epitope prediction and its application to global antibody-antigen docking. *Bioinformatics*, **2014**, 30, 2288-94	7.2	86
178	SAbPred: a structure-based antibody prediction server. *Nucleic Acids Research*, **2016**, 44, W474-8	20.1	79
177	Carbonyl-carbonyl interactions stabilize the partially allowed Ramachandran conformations of asparagine and aspartic acid. *Protein Engineering, Design and Selection*, **1999**, 12, 1025-8	1.9	79
176	Progress and challenges in predicting protein interfaces. *Briefings in Bioinformatics*, **2016**, 17, 117-31	13.4	78
175	Misato Controls Mitotic Microtubule Generation by Stabilizing the TCP-1 Tubulin Chaperone Complex. *Current Biology*, **2015**, 25, 2063	6.3	78
174	Rapid, Precise, and Reproducible Prediction of Peptide-MHC Binding Affinities from Molecular Dynamics That Correlate Well with Experiment. *Journal of Chemical Theory and Computation*, **2015**, 11, 3346-56	6.4	78
173	Solution structure and dynamics of a prototypical chordin-like cysteine-rich repeat (von Willebrand Factor type C module) from collagen IIA. *Journal of Biological Chemistry*, **2004**, 279, 53857-66	5.4	75
172	Association between a common immunoglobulin heavy chain allele and rheumatic heart disease risk in Oceania. *Nature Communications*, **2017**, 8, 14946	17.4	74
171	Observed Antibody Space: A Resource for Data Mining Next-Generation Sequencing of Antibody Repertoires. *Journal of Immunology*, **2018**, 201, 2502-2509	5.3	73
170	The function of communities in protein interaction networks at multiple scales. *BMC Systems Biology*, **2010**, 4, 100	3.5	63
169	Protein Family-Specific Models Using Deep Neural Networks and Transfer Learning Improve Virtual Screening and Highlight the Need for More Data. *Journal of Chemical Information and Modeling*, **2018**, 58, 2319-2330	6.1	63
168	Deciphering chemotaxis pathways using cross species comparisons. *BMC Systems Biology*, **2010**, 4, 3	3.5	57
167	Antibody i-Patch prediction of the antibody binding site improves rigid local antibody-antigen docking. *Protein Engineering, Design and Selection*, **2013**, 26, 621-9	1.9	55
166	How old is your fold?. *Bioinformatics*, **2005**, 21 Suppl 1, i449-58	7.2	55
165	Type II Inhibitors Targeting CDK2. *ACS Chemical Biology*, **2015**, 10, 2116-25	4.9	53
164	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
163	The H3 loop of antibodies shows unique structural characteristics. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 1311-1318	4.2	52

162	Helix kinks are equally prevalent in soluble and membrane proteins. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 1960-70	4.2	52
161	Deep Generative Models for 3D Linker Design. *Journal of Chemical Information and Modeling*, **2020**, 60, 1983-1995	6.1	49
160	Protein protein interactions, evolutionary rate, abundance and age. *BMC Bioinformatics*, **2006**, 7, 128	3.6	49
159	Identifying and quantifying radiation damage at the atomic level. *Journal of Synchrotron Radiation*, **2015**, 22, 201-12	2.4	41
158	Prediction of VH-VL domain orientation for antibody variable domain modeling. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 681-95	4.2	38
157	Deep Sequencing of B Cell Receptor Repertoires From COVID-19 Patients Reveals Strong Convergent Immune Signatures. *Frontiers in Immunology*, **2020**, 11, 605170	8.4	38
156	Predicting antibody complementarity determining region structures without classification. *Molecular BioSystems*, **2011**, 7, 3327-34		35
155	Predicting protein-protein interactions in the context of protein evolution. *Molecular BioSystems*, **2010**, 6, 55-64		34
154	Thera-SAbDab: the Therapeutic Structural Antibody Database. *Nucleic Acids Research*, **2020**, 48, D383-D388	20.1	34
153	Alignment-free protein interaction network comparison. *Bioinformatics*, **2014**, 30, i430-7	7.2	32
152	Memoir: template-based structure prediction for membrane proteins. *Nucleic Acids Research*, **2013**, 41, W379-83	20.1	32
151	Proteomic analysis of microtubule-associated proteins during macrophage activation. *Molecular and Cellular Proteomics*, **2009**, 8, 2500-14	7.6	32
150	Current status and future challenges in T-cell receptor/peptide/MHC molecular dynamics simulations. *Briefings in Bioinformatics*, **2015**, 16, 1035-44	13.4	31
149	Antibody H3 Structure Prediction. *Computational and Structural Biotechnology Journal*, **2017**, 15, 222-231	6.8	30
148	STCRDab: the structural T-cell receptor database. *Nucleic Acids Research*, **2018**, 46, D406-D412	20.1	30
147	Length-independent structural similarities enrich the antibody CDR canonical class model. *MAbs*, **2016**, 8, 751-60	6.6	30
146	Improved protein loop prediction from sequence alone. *Protein Engineering, Design and Selection*, **2001**, 14, 473-8	1.9	30
145	The Caenorhabditis elegans protein SAS-5 forms large oligomeric assemblies critical for centriole formation. *ELife*, **2015**, 4, e07410	8.9	30

144	How B-Cell Receptor Repertoire Sequencing Can Be Enriched with Structural Antibody Data. *Frontiers in Immunology*, **2017**, 8, 1753	8.4	29
143	An iterative structure-assisted approach to sequence alignment and comparative modeling **1999**, 37, 55-60		29
142	MP-T: improving membrane protein alignment for structure prediction. *Bioinformatics*, **2013**, 29, 54-61	7.2	28
141	Large scale characterization of the LC13 TCR and HLA-B8 structural landscape in reaction to 172 altered peptide ligands: a molecular dynamics simulation study. *PLoS Computational Biology*, **2014**, 10, e1003748	5	28
140	iMembrane: homology-based membrane-insertion of proteins. *Bioinformatics*, **2009**, 25, 1086-8	7.2	28
139	The prospects of quantum computing in computational molecular biology. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1481	7.9	28
138	What evidence is there for the homology of protein-protein interactions?. *PLoS Computational Biology*, **2012**, 8, e1002645	5	27
137	Cotranslational protein folding--fact or fiction?. *Bioinformatics*, **2007**, 23, i142-8	7.2	27
136	Functionally guided alignment of protein interaction networks for module detection. *Bioinformatics* , **2009**, 25, 3166-73	7.2	26
135	Sphinx: merging knowledge-based and ab initio approaches to improve protein loop prediction. *Bioinformatics*, **2017**, 33, 1346-1353	7.2	25
134	Structurally Mapping Antibody Repertoires. *Frontiers in Immunology*, **2018**, 9, 1698	8.4	25
133	Learning from the ligand: using ligand-based features to improve binding affinity prediction. *Bioinformatics*, **2020**, 36, 758-764	7.2	25
132	Fold usage on genomes and protein fold evolution. *Proteins: Structure, Function and Bioinformatics*, **2005**, 60, 690-700	4.2	25
131	The role and predicted propensity of conserved proline residues in the 5-HT3 receptor. *Journal of Biological Chemistry*, **2001**, 276, 37962-6	5.4	25
130	Exploring fold space preferences of new-born and ancient protein superfamilies. *PLoS Computational Biology*, **2013**, 9, e1003325	5	24
129	i-Patch: interprotein contact prediction using local network information. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2781-97	4.2	24
128	Modelling sequential protein folding under kinetic control. *Bioinformatics*, **2006**, 22, e203-10	7.2	23
127	How threshold behaviour affects the use of subgraphs for network comparison. *Bioinformatics*, **2010**, 26, i611-7	7.2	21

126	Predicting and validating protein interactions using network structure. *PLoS Computational Biology*, **2008**, 4, e1000118	5	21
125	Examining variable domain orientations in antigen receptors gives insight into TCR-like antibody design. *PLoS Computational Biology*, **2014**, 10, e1003852	5	20
124	How repertoire data are changing antibody science. *Journal of Biological Chemistry*, **2020**, 295, 9823-9837	5.4	19
123	Environment specific substitution tables improve membrane protein alignment. *Bioinformatics*, **2011**, 27, i15-23	7.2	19
122	A structural model of the human thrombopoietin receptor complex. *Journal of Molecular Graphics and Modelling*, **1997**, 15, 170-8, 185-8	2.8	18
121	An assessment of the uses of homologous interactions. *Bioinformatics*, **2008**, 24, 689-95	7.2	18
120	Examining the Conservation of Kinks in Alpha Helices. *PLoS ONE*, **2016**, 11, e0157553	3.7	17
119	SCALOP: sequence-based antibody canonical loop structure annotation. *Bioinformatics*, **2019**, 35, 1774-1776	7.26	17
118	Antibody–antigen complex modelling in the era of immunoglobulin repertoire sequencing. *Molecular Systems Design and Engineering*, **2019**, 4, 679-688	4.6	16
117	Exploring peptide/MHC detachment processes using hierarchical natural move Monte Carlo. *Bioinformatics*, **2016**, 32, 181-6	7.2	16
116	T-Cell Receptor Binding Affects the Dynamics of the Peptide/MHC-I Complex. *Journal of Chemical Information and Modeling*, **2016**, 56, 46-53	6.1	16
115	Partial-occupancy binders identified by the Pan-Dataset Density Analysis method offer new chemical opportunities and reveal cryptic binding sites. *Structural Dynamics*, **2017**, 4, 032104	3.2	16
114	Building a better fragment library for de novo protein structure prediction. *PLoS ONE*, **2015**, 10, e0123998	3.7	16
113	The imprint of codons on protein structure. *Biotechnology Journal*, **2011**, 6, 641-9	5.6	16
112	Looking for therapeutic antibodies in next-generation sequencing repositories. *MAbs*, **2019**, 11, 1197-1205	6.5	15
111	Structural diversity of B-cell receptor repertoires along the B-cell differentiation axis in humans and mice. *PLoS Computational Biology*, **2020**, 16, e1007636	5	15
110	Predicting loop conformational ensembles. *Bioinformatics*, **2018**, 34, 949-956	7.2	15
109	Gro2mat: a package to efficiently read gromacs output in MATLAB. *Journal of Computational Chemistry*, **2014**, 35, 1528-31	3.5	15

108	Co-evolution techniques are reshaping the way we do structural bioinformatics. *F1000Research*, **2017**, 6, 1224	3.6	15
107	Producing high-accuracy lattice models from protein atomic coordinates including side chains. *Advances in Bioinformatics*, **2012**, 2012, 148045	5.5	15
106	Directionality in protein fold prediction. *BMC Bioinformatics*, **2010**, 11, 172	3.6	15
105	Data Set Augmentation Allows Deep Learning-Based Virtual Screening to Better Generalize to Unseen Target Classes and Highlight Important Binding Interactions. *Journal of Chemical Information and Modeling*, **2020**, 60, 3722-3730	6.1	15
104	Computational Tools for Aiding Rational Antibody Design. *Methods in Molecular Biology*, **2017**, 1529, 399-416	1.4	14
103	Measuring rank robustness in scored protein interaction networks. *BMC Bioinformatics*, **2019**, 20, 446	3.6	14
102	The contribution of major histocompatibility complex contacts to the affinity and kinetics of T cell receptor binding. *Scientific Reports*, **2016**, 6, 35326	4.9	14
101	Misato Controls Mitotic Microtubule Generation by Stabilizing the TCP-1 Tubulin Chaperone Complex [corrected]. *Current Biology*, **2015**, 25, 1777-83	6.3	14
100	Protein structure prediction begins well but ends badly. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1282-90	4.2	14
99	Maturation of the Human Immunoglobulin Heavy Chain Repertoire With Age. *Frontiers in Immunology*, **2020**, 11, 1734	8.4	14
98	Comparing co-evolution methods and their application to template-free protein structure prediction. *Bioinformatics*, **2017**, 33, 373-381	7.2	14
97	Comparative Analysis of the CDR Loops of Antigen Receptors. *Frontiers in Immunology*, **2019**, 10, 2454	8.4	13
96	Cross-linking mass spectrometry identifies new interfaces of Augmin required to localise the γ-tubulin ring complex to the mitotic spindle. *Biology Open*, **2017**, 6, 654-663	2.2	13
95	Humanization of antibodies using a machine learning approach on large-scale repertoire data. *Bioinformatics*, **2021**,	7.2	13
94	Variable Regions of Antibodies and T-Cell Receptors May Not Be Sufficient in Molecular Simulations Investigating Binding. *Journal of Chemical Theory and Computation*, **2017**, 13, 3097-3105	6.4	12
93	Identifying networks with common organizational principles. *Journal of Complex Networks*, **2018**, 6, 887-917	2.3	12
92	Antibody side chain conformations are position-dependent. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86, 383-392	4.2	12
91	ABlooper: Fast accurate antibody CDR loop structure prediction with accuracy estimation.. *Bioinformatics*, **2022**,	7.2	12

90	Structural Bridges through Fold Space. *PLoS Computational Biology*, **2015**, 11, e1004466	5	11
89	The importance of age and high degree, in protein-protein interaction networks. *Journal of Computational Biology*, **2012**, 19, 785-95	1.7	11
88	Signatures of co-translational folding. *Biotechnology Journal*, **2011**, 6, 742-51	5.6	11
87	Deep sequencing of B cell receptor repertoires from COVID-19 patients reveals strong convergent immune signatures		11
86	A computational method for immune repertoire mining that identifies novel binders from different clonotypes, demonstrated by identifying anti-pertussis toxoid antibodies. *MAbs*, **2021**, 13, 1869406	6.6	11
85	Exploring the potential of template-based modelling. *Bioinformatics*, **2010**, 26, 1849-56	7.2	10
84	CoV-AbDab: the Coronavirus Antibody Database		10
83	OOMMPPAA: a tool to aid directed synthesis by the combined analysis of activity and structural data. *Journal of Chemical Information and Modeling*, **2014**, 54, 2636-46	6.1	9
82	Evolutionary analysis reveals low coverage as the major challenge for protein interaction network alignment. *Molecular BioSystems*, **2010**, 6, 2296-304		9
81	Ab-Ligity: identifying sequence-dissimilar antibodies that bind to the same epitope. *MAbs*, **2021**, 13, 1873478	6.6	9
80	Filtering Next-Generation Sequencing of the Ig Gene Repertoire Data Using Antibody Structural Information. *Journal of Immunology*, **2018**, 201, 3694-3704	5.3	9
79	Ligity: A Non-Superpositional, Knowledge-Based Approach to Virtual Screening. *Journal of Chemical Information and Modeling*, **2019**, 59, 2600-2616	6.1	8
78	How long is a piece of loop?. *PeerJ*, **2013**, 1, e1	3.1	8
77	Public Baseline and shared response structures support the theory of antibody repertoire functional commonality. *PLoS Computational Biology*, **2021**, 17, e1008781	5	8
76	MHC binding affects the dynamics of different T-cell receptors in different ways. *PLoS Computational Biology*, **2019**, 15, e1007338	5	8
75	Sequential search leads to faster, more efficient fragment-based de novo protein structure prediction. *Bioinformatics*, **2018**, 34, 1132-1140	7.2	8
74	DLAB-Deep learning methods for structure-based virtual screening of antibodies. *Bioinformatics*, **2021**,	7.2	8
73	Functional module detection through integration of single-cell RNA sequencing data with protein-protein interaction networks. *BMC Genomics*, **2020**, 21, 756	4.5	7

72	Comparison of large networks with sub-sampling strategies. *Scientific Reports*, **2016**, 6, 28955	4.9	7
71	Fragment-based modeling of membrane protein loops: successes, failures, and prospects for the future. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 175-86	4.2	7
70	Observed Antibody Space: A diverse database of cleaned, annotated, and translated unpaired and paired antibody sequences. *Protein Science*, **2021**,	6.3	7
69	Modeling conformational flexibility of kinases in inactive states. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 943-951	4.2	6
68	Combining co-evolution and secondary structure prediction to improve fragment library generation. *Bioinformatics*, **2018**, 34, 2219-2227	7.2	6
67	Crowdsourcing yields a new standard for kinks in protein helices. *Journal of Chemical Information and Modeling*, **2014**, 54, 2585-93	6.1	6
66	Current advances in biopharmaceutical informatics: guidelines, impact and challenges in the computational developability assessment of antibody therapeutics.. *MAbs*, **2022**, 14, 2020082	6.6	6
65	Epitope profiling using computational structural modelling demonstrated on coronavirus-binding antibodies.. *PLoS Computational Biology*, **2021**, 17, e1009675	5	6
64	Deep generative design with 3D pharmacophoric constraints. *Chemical Science*, **2021**, 12, 14577-14589	9.4	6
63	Modeling Functional Motions of Biological Systems by Customized Natural Moves. *Biophysical Journal*, **2016**, 111, 710-721	2.9	6
62	Local network patterns in protein-protein interfaces. *PLoS ONE*, **2013**, 8, e57031	3.7	5
61	Protein three-dimensional structural databases: domains, structurally aligned homologues and superfamilies. *Acta Crystallographica Section D: Biological Crystallography*, **1998**, 54, 1168-77		5
60	A statistical approach using network structure in the prediction of protein characteristics. *Bioinformatics*, **2007**, 23, 2314-21	7.2	5
59	A Multi-Crystal Method for Extracting Obscured Signal from Crystallographic Electron Density		5
58	Epitope profiling of coronavirus-binding antibodies using computational structural modelling		5
57	Hypergraphs for predicting essential genes using multiprotein complex data. *Journal of Complex Networks*, **2021**, 9,	1.7	5
56	Tertiary Element Interaction in HIV-1 TAR. *Journal of Chemical Information and Modeling*, **2016**, 56, 1746-54		5
55	The allosteric modulation of complement C5 by knob domain peptides. *ELife*, **2021**, 10,	8.9	5

54	TCRBuilder: multi-state T-cell receptor structure prediction. *Bioinformatics*, **2020**, 36, 3580-3581	7.2	4
53	pyHVis3D: visualising molecular simulation deduced H-bond networks in 3D: application to T-cell receptor interactions. *Bioinformatics*, **2018**, 34, 1941-1943	7.2	4
52	The functional domain grouping of microtubule associated proteins. *Communicative and Integrative Biology*, **2008**, 1, 47-50	1.7	4
51	Using phylogeny to improve genome-wide distant homology recognition. *PLoS Computational Biology*, **2007**, 3, e3	5	4
50	Evidence of Antibody Repertoire Functional Convergence through Public Baseline and Shared Response Structures		4
49	SAbDab in the age of biotherapeutics: updates including SAbDab-nano, the nanobody structure tracker.. *Nucleic Acids Research*, **2022**, 50, D1368-D1372	20.1	4
48	Different B cell subpopulations show distinct patterns in their IgH repertoire metrics. *ELife*, **2021**, 10,	8.9	4
47	Maturation of the human B-cell receptor repertoire with age		4
46	Comparative analysis of the CDR loops of antigen receptors		4
45	Structural Diversity of B-Cell Receptor Repertoires along the B-cell Differentiation Axis in Humans and Mice		4
44	Robust gene coexpression networks using signed distance correlation. *Bioinformatics*, **2021**,	7.2	4
43	Co-evolutionary Distance Predictions Contain Flexibility Information. *Bioinformatics*, **2021**,	7.2	4
42	In silico structural modeling of multiple epigenetic marks on DNA. *Bioinformatics*, **2018**, 34, 41-48	7.2	3
41	RFQAmodel: Random Forest Quality Assessment to identify a predicted protein structure in the correct fold. *PLoS ONE*, **2019**, 14, e0218149	3.7	3
40	Mutual information and variants for protein domain-domain contact prediction. *BMC Research Notes*, **2012**, 5, 472	2.3	3
39	Protein Interaction Networks and Their Statistical Analysis **2011**, 200-234		3
38	Current structure predictors are not learning the physics of protein folding.. *Bioinformatics*, **2022**,	7.2	3
37	WONKA and OOMMPPAA: analysis of protein-ligand interaction data to direct structure-based drug design. *Acta Crystallographica Section D: Structural Biology*, **2017**, 73, 279-285	5.5	3

36	Ab-Ligity: Identifying sequence-dissimilar antibodies that bind to the same epitope		3
35	Increasing the accuracy of protein loop structure prediction with evolutionary constraints. *Bioinformatics*, **2019**, 35, 2585-2592	7.2	3
34	Generating Property-Matched Decoy Molecules Using Deep Learning. *Bioinformatics*, **2021**,	7.2	3
33	DLAB - Deep learning methods for structure-based virtual screening of antibodies		3
32	A statistical model for helices with applications. *Biometrics*, **2018**, 74, 845-854	1.8	2
31	The evolution of contact prediction: evidence that contact selection in statistical contact prediction is changing. *Bioinformatics*, **2020**, 36, 1750-1756	7.2	2
30	Predicting inter-species cross-talk in two-component signalling systems. *PLoS ONE*, **2012**, 7, e37737	3.7	2
29	Current strategies for detecting functional convergence across B-cell receptor repertoires. *MAbs*, **2021**, 13, 1996732	6.6	2
28	Functional module detection through integration of single-cell RNA sequencing data with protein□protein interaction networks		2
27	COGENT: evaluating the consistency of gene co-expression networks. *Bioinformatics*, **2021**, 37, 1928-1929	7.2	2
26	Ribosome occupancy profiles are conserved between structurally and evolutionarily related yeast domains. *Bioinformatics*, **2021**,	7.2	2
25	Investigating the potential for a limited quantum speedup on protein lattice problems. *New Journal of Physics*,	2.9	2
24	Current protein structure predictors do not produce meaningful folding pathways		2
23	Humanization of antibodies using a machine learning approach on large-scale repertoire data		2
22	HLA-DM Stabilizes the Empty MHCII Binding Groove: A Model Using Customized Natural Move Monte Carlo. *Journal of Chemical Information and Modeling*, **2019**, 59, 2894-2899	6.1	1
21	Protein Modeling and Structural Prediction **2014**, 171-182		1
20	Incorporating Target-Specific Pharmacophoric Information Into Deep Generative Models For Fragment Elaboration		1
19	Measuring rank robustness in scored protein interaction networks		1

18	A computational method for immune repertoire mining that identifies novel binders from different clonotypes, demonstrated by identifying anti-Pertussis toxoid antibodies		1
17	PROTEIN COMPARATIVE MODELLING AND DRUG DISCOVERY **2003**, 445-458		1
16	Novel Vβ-specific germline contacts shape an elite controller T cell response		1
15	Co-evolutionary Distance Prediction for Flexibility Prediction		1
14	Looking for Therapeutic Antibodies in Next Generation Sequencing Repositories		1
13	Deep Generative Design with 3D Pharmacophoric Constraints		1
12	High-Throughput Antibody Structure Modeling and Design Using ABodyBuilder. *Methods in Molecular Biology*, **2019**, 1851, 367-380	1.4	1
11	ABlooper: Fast accurate antibody CDR loop structure prediction with accuracy estimation		1
10	Assessment of model fit via network comparison methods based on subgraph counts. *Journal of Complex Networks*, **2019**, 7, 226-253	1.7	0
9	AI in 3D compound design.. *Current Opinion in Structural Biology*, **2022**, 73, 102326	8.1	0
8	The Therapeutic Antibody Profiler for Computational Developability Assessment. *Methods in Molecular Biology*, **2022**, 2313, 115-125	1.4	0
7	Membranome 3.0: Database of single-pass membrane proteins with AlphaFold models.. *Protein Science*, **2022**, 31, e4318	6.3	0
6	Advances in computational structure-based antibody design.. *Current Opinion in Structural Biology*, **2022**, 74, 102379	8.1	0
5	Ranking of communities in multiplex spatiotemporal models of brain dynamics.. *Applied Network Science*, **2022**, 7, 15	2.9	
4	Structural diversity of B-cell receptor repertoires along the B-cell differentiation axis in humans and mice **2020**, 16, e1007636		
3	Structural diversity of B-cell receptor repertoires along the B-cell differentiation axis in humans and mice **2020**, 16, e1007636		
2	Structural diversity of B-cell receptor repertoires along the B-cell differentiation axis in humans and mice **2020**, 16, e1007636		
1	Structural diversity of B-cell receptor repertoires along the B-cell differentiation axis in humans and mice **2020**, 16, e1007636		