

# Charlotte M Deane

## List of Publications by Year in descending order

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Version: 2024-02-01

189  
papers

9,609  
citations

57631

44  
h-index

58464

82  
g-index

290  
all docs

290  
docs citations

290  
times ranked

10289  
citing authors

#	ARTICLE	IF	CITATIONS
1	Protein Interactions. <i>Molecular and Cellular Proteomics</i> , 2002, 1, 349-356.	2.5	570
2	HOMSTRAD: A database of protein structure alignments for homologous families. <i>Protein Science</i> , 1998, 7, 2469-2471.	3.1	461
3	SAbDab: the structural antibody database. <i>Nucleic Acids Research</i> , 2014, 42, D1140-D1146.	6.5	374
4	CoV-AbDab: the coronavirus antibody database. <i>Bioinformatics</i> , 2021, 37, 734-735.	1.8	273
5	Reduced amounts and abnormal forms of phospholipase C zeta (PLC $\zeta$ ) in spermatozoa from infertile men. <i>Human Reproduction</i> , 2009, 24, 2417-2428.	0.4	257
6	ANARCI: antigen receptor numbering and receptor classification. <i>Bioinformatics</i> , 2016, 32, 298-300.	1.8	237
7	Five computational developability guidelines for therapeutic antibody profiling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 4025-4030.	3.3	221
8	ABodyBuilder: Automated antibody structure prediction with data-driven accuracy estimation. <i>MAbs</i> , 2016, 8, 1259-1268.	2.6	208
9	Avoiding False Positive Conclusions in Molecular Simulation: The Importance of Replicas. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6127-6138.	2.3	187
10	A multi-crystal method for extracting obscured crystallographic states from conventionally uninterpretable electron density. <i>Nature Communications</i> , 2017, 8, 15123.	5.8	186
11	Freely Available Conformer Generation Methods: How Good Are They?. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1146-1158.	2.5	178
12	Observed Antibody Space: A Resource for Data Mining Next-Generation Sequencing of Antibody Repertoires. <i>Journal of Immunology</i> , 2018, 201, 2502-2509.	0.4	165
13	SAbPred: a structure-based antibody prediction server. <i>Nucleic Acids Research</i> , 2016, 44, W474-W478.	6.5	155
14	FREAD revisited: Accurate loop structure prediction using a database search algorithm. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 1431-1440.	1.5	154
15	Synonymous codon usage influences the local protein structure observed. <i>Nucleic Acids Research</i> , 2010, 38, 6719-6728.	6.5	148
16	CODA: A combined algorithm for predicting the structurally variable regions of protein models. <i>Protein Science</i> , 2001, 10, 599-612.	3.1	147
17	Improving B-cell epitope prediction and its application to global antibody-antigen docking. <i>Bioinformatics</i> , 2014, 30, 2288-2294.	1.8	137
18	Revisiting Date and Party Hubs: Novel Approaches to Role Assignment in Protein Interaction Networks. <i>PLoS Computational Biology</i> , 2010, 6, e1000817.	1.5	128

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19	Deep Generative Models for 3D Linker Design. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1983-1995.	2.5	126
20	Rapid, Precise, and Reproducible Prediction of Peptide-MHC Binding Affinities from Molecular Dynamics That Correlate Well with Experiment. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3346-3356.	2.3	122
21	A maternally inherited autosomal point mutation in human phospholipase C zeta (PLC $\zeta$ ) leads to male infertility. <i>Human Reproduction</i> , 2012, 27, 222-231.	0.4	117
22	Progress and challenges in predicting protein interfaces. <i>Briefings in Bioinformatics</i> , 2016, 17, 117-131.	3.2	115
23	Association between a common immunoglobulin heavy chain allele and rheumatic heart disease risk in Oceania. <i>Nature Communications</i> , 2017, 8, 14946.	5.8	114
24	The prospects of quantum computing in computational molecular biology. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1481.	6.2	108
25	Protein Family-Specific Models Using Deep Neural Networks and Transfer Learning Improve Virtual Screening and Highlight the Need for More Data. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 2319-2330.	2.5	106
26	A Microtubule Interactome: Complexes with Roles in Cell Cycle and Mitosis. <i>PLoS Biology</i> , 2008, 6, e98.	2.6	105
27	MEDELLER: homology-based coordinate generation for membrane proteins. <i>Bioinformatics</i> , 2010, 26, 2833-2840.	1.8	103
28	Deep Sequencing of B Cell Receptor Repertoires From COVID-19 Patients Reveals Strong Convergent Immune Signatures. <i>Frontiers in Immunology</i> , 2020, 11, 605170.	2.2	101
29	Observed Antibody Space: A diverse database of cleaned, annotated, and translated unpaired and paired antibody sequences. <i>Protein Science</i> , 2022, 31, 141-146.	3.1	98
30	Carbonyl-carbonyl interactions stabilize the partially allowed Ramachandran conformations of asparagine and aspartic acid. <i>Protein Engineering, Design and Selection</i> , 1999, 12, 1025-1028.	1.0	90
31	The H3 loop of antibodies shows unique structural characteristics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1311-1318.	1.5	89
32	Thera-SAbDab: the Therapeutic Structural Antibody Database. <i>Nucleic Acids Research</i> , 2020, 48, D383-D388.	6.5	88
33	Solution Structure and Dynamics of a Prototypical Chordin-like Cysteine-rich Repeat (von Willebrand) Tj ETQq1 1 0,784314 rgBT /Ove	1.6	83
34	Antibody i-Patch prediction of the antibody binding site improves rigid local antibody-antigen docking. <i>Protein Engineering, Design and Selection</i> , 2013, 26, 621-629.	1.0	80
35	The function of communities in protein interaction networks at multiple scales. <i>BMC Systems Biology</i> , 2010, 4, 100.	3.0	79
36	ABlooper: fast accurate antibody CDR loop structure prediction with accuracy estimation. <i>Bioinformatics</i> , 2022, 38, 1877-1880.	1.8	78

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37	Type II Inhibitors Targeting CDK2. <i>ACS Chemical Biology</i> , 2015, 10, 2116-2125.	1.6	75
38	STCRDab: the structural T-cell receptor database. <i>Nucleic Acids Research</i> , 2018, 46, D406-D412.	6.5	69
39	Deciphering chemotaxis pathways using cross species comparisons. <i>BMC Systems Biology</i> , 2010, 4, 3.	3.0	66
40	Protein protein interactions, evolutionary rate, abundance and age. <i>BMC Bioinformatics</i> , 2006, 7, 128.	1.2	64
41	How old is your fold?. <i>Bioinformatics</i> , 2005, 21, i449-i458.	1.8	63
42	Helix kinks are equally prevalent in soluble and membrane proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 1960-1970.	1.5	61
43	A novel exhaustive search algorithm for predicting the conformation of polypeptide segments in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000, 40, 135-144.	1.5	60
44	Learning from the ligand: using ligand-based features to improve binding affinity prediction. <i>Bioinformatics</i> , 2020, 36, 758-764.	1.8	60
45	Identifying and quantifying radiation damage at the atomic level. <i>Journal of Synchrotron Radiation</i> , 2015, 22, 201-212.	1.0	51
46	Current structure predictors are not learning the physics of protein folding. <i>Bioinformatics</i> , 2022, 38, 1881-1887.	1.8	50
47	Length-independent structural similarities enrich the antibody CDR canonical class model. <i>MAbs</i> , 2016, 8, 751-760.	2.6	49
48	Sphinx: merging knowledge-based and <i>ab initio</i> approaches to improve protein loop prediction. <i>Bioinformatics</i> , 2017, 33, 1346-1353.	1.8	49
49	Humanization of antibodies using a machine learning approach on large-scale repertoire data. <i>Bioinformatics</i> , 2021, 37, 4041-4047.	1.8	49
50	SAbDab in the age of biotherapeutics: updates including SAbDab-nano, the nanobody structure tracker. <i>Nucleic Acids Research</i> , 2022, 50, D1368-D1372.	6.5	49
51	Alignment-free protein interaction network comparison. <i>Bioinformatics</i> , 2014, 30, i430-i437.	1.8	48
52	How B-Cell Receptor Repertoire Sequencing Can Be Enriched with Structural Antibody Data. <i>Frontiers in Immunology</i> , 2017, 8, 1753.	2.2	48
53	DLAB: deep learning methods for structure-based virtual screening of antibodies. <i>Bioinformatics</i> , 2022, 38, 377-383.	1.8	48
54	AbLang: an antibody language model for completing antibody sequences. <i>Bioinformatics Advances</i> , 2022, 2, .	0.9	48

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55	Ten Simple Rules for Effective Computational Research. <i>PLoS Computational Biology</i> , 2014, 10, e1003506.	1.5	47
56	Prediction of VH-VL domain orientation for antibody variable domain modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 681-695.	1.5	47
57	Antibody H3 Structure Prediction. <i>Computational and Structural Biotechnology Journal</i> , 2017, 15, 222-231.	1.9	47
58	Ten Simple Rules for a Successful Cross-Disciplinary Collaboration. <i>PLoS Computational Biology</i> , 2015, 11, e1004214.	1.5	46
59	Maturation of the Human Immunoglobulin Heavy Chain Repertoire With Age. <i>Frontiers in Immunology</i> , 2020, 11, 1734.	2.2	46
60	Current status and future challenges in T-cell receptor/peptide/MHC molecular dynamics simulations. <i>Briefings in Bioinformatics</i> , 2015, 16, 1035-1044.	3.2	45
61	How repertoire data are changing antibody science. <i>Journal of Biological Chemistry</i> , 2020, 295, 9823-9837.	1.6	43
62	Predicting protein-protein interactions in the context of protein evolution. <i>Molecular BioSystems</i> , 2010, 6, 55-64.	2.9	42
63	Proteomic Analysis of Microtubule-associated Proteins during Macrophage Activation. <i>Molecular and Cellular Proteomics</i> , 2009, 8, 2500-2514.	2.5	41
64	What Evidence Is There for the Homology of Protein-Protein Interactions?. <i>PLoS Computational Biology</i> , 2012, 8, e1002645.	1.5	41
65	Comparative Analysis of the CDR Loops of Antigen Receptors. <i>Frontiers in Immunology</i> , 2019, 10, 2454.	2.2	40
66	Predicting antibody complementarity determining region structures without classification. <i>Molecular BioSystems</i> , 2011, 7, 3327.	2.9	39
67	Memoir: template-based structure prediction for membrane proteins. <i>Nucleic Acids Research</i> , 2013, 41, W379-W383.	6.5	38
68	The <i>Caenorhabditis elegans</i> protein SAS-5 forms large oligomeric assemblies critical for centriole formation. <i>ELife</i> , 2015, 4, e07410.	2.8	37
69	Structurally Mapping Antibody Repertoires. <i>Frontiers in Immunology</i> , 2018, 9, 1698.	2.2	36
70	Data Set Augmentation Allows Deep Learning-Based Virtual Screening to Better Generalize to Unseen Target Classes and Highlight Important Binding Interactions. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3722-3730.	2.5	36
71	Deep generative design with 3D pharmacophoric constraints. <i>Chemical Science</i> , 2021, 12, 14577-14589.	3.7	36
72	The Role and Predicted Propensity of Conserved Proline Residues in the 5-HT3 Receptor. <i>Journal of Biological Chemistry</i> , 2001, 276, 37962-37966.	1.6	35

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73	Current advances in biopharmaceutical informatics: guidelines, impact and challenges in the computational developability assessment of antibody therapeutics. <i>MABs</i> , 2022, 14, 2020082.	2.6	35
74	Epitope profiling using computational structural modelling demonstrated on coronavirus-binding antibodies. <i>PLoS Computational Biology</i> , 2021, 17, e1009675.	1.5	33
75	An iterative structure-assisted approach to sequence alignment and comparative modeling. , 1999, 37, 55-60.		32
76	Improved protein loop prediction from sequence alone. <i>Protein Engineering, Design and Selection</i> , 2001, 14, 473-478.	1.0	32
77	Large Scale Characterization of the LC13 TCR and HLA-B8 Structural Landscape in Reaction to 172 Altered Peptide Ligands: A Molecular Dynamics Simulation Study. <i>PLoS Computational Biology</i> , 2014, 10, e1003748.	1.5	32
78	Advances in computational structure-based antibody design. <i>Current Opinion in Structural Biology</i> , 2022, 74, 102379.	2.6	32
79	Functionally guided alignment of protein interaction networks for module detection. <i>Bioinformatics</i> , 2009, 25, 3166-3173.	1.8	31
80	Exploring Fold Space Preferences of New-born and Ancient Protein Superfamilies. <i>PLoS Computational Biology</i> , 2013, 9, e1003325.	1.5	31
81	Ab-Ligity: identifying sequence-dissimilar antibodies that bind to the same epitope. <i>MABs</i> , 2021, 13, 1873478.	2.6	31
82	A computational method for immune repertoire mining that identifies novel binders from different clonotypes, demonstrated by identifying anti-pertussis toxoid antibodies. <i>MABs</i> , 2021, 13, 1869406.	2.6	31
83	Fold usage on genomes and protein fold evolution. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 60, 690-700.	1.5	30
84	Predicting and Validating Protein Interactions Using Network Structure. <i>PLoS Computational Biology</i> , 2008, 4, e1000118.	1.5	30
85	MP-T: improving membrane protein alignment for structure prediction. <i>Bioinformatics</i> , 2013, 29, 54-61.	1.8	30
86	Measuring rank robustness in scored protein interaction networks. <i>BMC Bioinformatics</i> , 2019, 20, 446.	1.2	30
87	Generating property-matched decoy molecules using deep learning. <i>Bioinformatics</i> , 2021, 37, 2134-2141.	1.8	30
88	iMembrane: homology-based membrane-insertion of proteins. <i>Bioinformatics</i> , 2009, 25, 1086-1088.	1.8	29
89	Examining Variable Domain Orientations in Antigen Receptors Gives Insight into TCR-Like Antibody Design. <i>PLoS Computational Biology</i> , 2014, 10, e1003852.	1.5	29
90	Looking for therapeutic antibodies in next-generation sequencing repositories. <i>MABs</i> , 2019, 11, 1197-1205.	2.6	29

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91	SCALOP: sequence-based antibody canonical loop structure annotation. <i>Bioinformatics</i> , 2019, 35, 1774-1776.	1.8	29
92	Cotranslational protein folding—fact or fiction?. <i>Bioinformatics</i> , 2007, 23, i142-i148.	1.8	28
93	Comparing co-evolution methods and their application to template-free protein structure prediction. <i>Bioinformatics</i> , 2017, 33, 373-381.	1.8	28
94	Structural diversity of B-cell receptor repertoires along the B-cell differentiation axis in humans and mice. <i>PLoS Computational Biology</i> , 2020, 16, e1007636.	1.5	27
95	iPatch: Interprotein contact prediction using local network information. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 2781-2797.	1.5	26
96	How threshold behaviour affects the use of subgraphs for network comparison. <i>Bioinformatics</i> , 2010, 26, i611-i617.	1.8	26
97	Public Baseline and shared response structures support the theory of antibody repertoire functional commonality. <i>PLoS Computational Biology</i> , 2021, 17, e1008781.	1.5	26
98	Building a Better Fragment Library for De Novo Protein Structure Prediction. <i>PLoS ONE</i> , 2015, 10, e0123998.	1.1	25
99	Misato Controls Mitotic Microtubule Generation by Stabilizing the TCP-1 Tubulin Chaperone Complex. <i>Current Biology</i> , 2015, 25, 1777-1783.	1.8	25
100	Partial-occupancy binders identified by the Pan-Dataset Density Analysis method offer new chemical opportunities and reveal cryptic binding sites. <i>Structural Dynamics</i> , 2017, 4, 032104.	0.9	25
101	Cross-linking mass spectrometry identifies new interfaces of Augmin required to localise the $\hat{\gamma}$ -Tubulin Ring Complex to the mitotic spindle. <i>Biology Open</i> , 2017, 6, 654-663.	0.6	25
102	Modelling sequential protein folding under kinetic control. <i>Bioinformatics</i> , 2006, 22, e203-e210.	1.8	23
103	An assessment of the uses of homologous interactions. <i>Bioinformatics</i> , 2008, 24, 689-695.	1.8	22
104	Producing High-Accuracy Lattice Models from Protein Atomic Coordinates Including Side Chains. <i>Advances in Bioinformatics</i> , 2012, 2012, 1-6.	5.7	22
105	Computational Tools for Aiding Rational Antibody Design. <i>Methods in Molecular Biology</i> , 2017, 1529, 399-416.	0.4	22
106	Co-evolution techniques are reshaping the way we do structural bioinformatics. <i>F1000Research</i> , 2017, 6, 1224.	0.8	22
107	Different B cell subpopulations show distinct patterns in their IgH repertoire metrics. <i>ELife</i> , 2021, 10, .	2.8	22
108	Exploring peptide/MHC detachment processes using hierarchical natural move Monte Carlo. <i>Bioinformatics</i> , 2016, 32, 181-186.	1.8	21

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109	T-Cell Receptor Binding Affects the Dynamics of the Peptide/MHC-I Complex. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 46-53.	2.5	21
110	Variable Regions of Antibodies and T-Cell Receptors May Not Be Sufficient in Molecular Simulations Investigating Binding. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3097-3105.	2.3	21
111	Antibody side chain conformations are position-dependent. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 383-392.	1.5	21
112	The allosteric modulation of complement C5 by knob domain peptides. <i>ELife</i> , 2021, 10, .	2.8	21
113	Environment specific substitution tables improve membrane protein alignment. <i>Bioinformatics</i> , 2011, 27, i15-i23.	1.8	20
114	Examining the Conservation of Kinks in Alpha Helices. <i>PLoS ONE</i> , 2016, 11, e0157553.	1.1	20
115	Identifying networks with common organizational principles. <i>Journal of Complex Networks</i> , 2018, 6, 887-913.	1.1	20
116	Predicting loop conformational ensembles. <i>Bioinformatics</i> , 2018, 34, 949-956.	1.8	20
117	Antibody-antigen complex modelling in the era of immunoglobulin repertoire sequencing. <i>Molecular Systems Design and Engineering</i> , 2019, 4, 679-688.	1.7	20
118	Membranome 3.0: Database of single-pass membrane proteins with AlphaFold models. <i>Protein Science</i> , 2022, 31, e4318.	3.1	20
119	A structural model of the human thrombopoietin receptor complex. <i>Journal of Molecular Graphics and Modelling</i> , 1997, 15, 170-188.	1.3	18
120	Gro2mat: A package to efficiently read gromacs output in MATLAB. <i>Journal of Computational Chemistry</i> , 2014, 35, 1528-1531.	1.5	18
121	The contribution of major histocompatibility complex contacts to the affinity and kinetics of T cell receptor binding. <i>Scientific Reports</i> , 2016, 6, 35326.	1.6	18
122	Current strategies for detecting functional convergence across B-cell receptor repertoires. <i>MAbs</i> , 2021, 13, 1996732.	2.6	18
123	Directionality in protein fold prediction. <i>BMC Bioinformatics</i> , 2010, 11, 172.	1.2	17
124	The imprint of codons on protein structure. <i>Biotechnology Journal</i> , 2011, 6, 641-649.	1.8	17
125	How long is a piece of loop?. <i>PeerJ</i> , 2013, 1, e1.	0.9	17
126	Structural Bridges through Fold Space. <i>PLoS Computational Biology</i> , 2015, 11, e1004466.	1.5	16



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127	Hypergraphs for predicting essential genes using multiprotein complex data. <i>Journal of Complex Networks</i> , 2021, 9, .	1.1	16
128	Protein structure prediction begins well but ends badly. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 1282-1290.	1.5	15
129	Signatures of coâ€translational folding. <i>Biotechnology Journal</i> , 2011, 6, 742-751.	1.8	15
130	Fragment-based modeling of membrane protein loops: Successes, failures, and prospects for the future. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 175-186.	1.5	15
131	MHC binding affects the dynamics of different T-cell receptors in different ways. <i>PLoS Computational Biology</i> , 2019, 15, e1007338.	1.5	13
132	Functional module detection through integration of single-cell RNA sequencing data with proteinâ€protein interaction networks. <i>BMC Genomics</i> , 2020, 21, 756.	1.2	13
133	Sequential search leads to faster, more efficient fragment-based <i>de novo</i> protein structure prediction. <i>Bioinformatics</i> , 2018, 34, 1132-1140.	1.8	12
134	Exploring the potential of template-based modelling. <i>Bioinformatics</i> , 2010, 26, 1849-1856.	1.8	11
135	Evolutionary analysis reveals low coverage as the major challenge for protein interaction network alignment. <i>Molecular BioSystems</i> , 2010, 6, 2296.	2.9	11
136	The Importance of Age and High Degree, in Protein-Protein Interaction Networks. <i>Journal of Computational Biology</i> , 2012, 19, 785-795.	0.8	11
137	Filtering Next-Generation Sequencing of the Ig Gene Repertoire Data Using Antibody Structural Information. <i>Journal of Immunology</i> , 2018, 201, 3694-3704.	0.4	11
138	Modeling conformational flexibility of kinases in inactive states. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 943-951.	1.5	11
139	TCRBuilder: multi-state T-cell receptor structure prediction. <i>Bioinformatics</i> , 2020, 36, 3580-3581.	1.8	10
140	Robust gene coexpression networks using signed distance correlation. <i>Bioinformatics</i> , 2021, 37, 1982-1989.	1.8	10
141	Learning from Docked Ligands: Ligand-Based Features Rescue Structure-Based Scoring Functions When Trained on Docked Poses. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 5329-5341.	2.5	10
142	Incorporating Target-Specific Pharmacophoric Information into Deep Generative Models for Fragment Elaboration. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2280-2292.	2.5	10
143	OOMPPAA: A Tool To Aid Directed Synthesis by the Combined Analysis of Activity and Structural Data. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2636-2646.	2.5	9
144	Comparison of large networks with sub-sampling strategies. <i>Scientific Reports</i> , 2016, 6, 28955.	1.6	9

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145	Ligity: A Non-Superpositional, Knowledge-Based Approach to Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2600-2616.	2.5	9
146	Co-evolutionary distance predictions contain flexibility information. <i>Bioinformatics</i> , 2021, , .	1.8	9
147	Tertiary Element Interaction in HIV-1 TAR. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1746-1754.	2.5	8
148	Increasing the accuracy of protein loop structure prediction with evolutionary constraints. <i>Bioinformatics</i> , 2019, 35, 2585-2592.	1.8	8
149	AI in 3D compound design. <i>Current Opinion in Structural Biology</i> , 2022, 73, 102326.	2.6	8
150	Crowdsourcing Yields a New Standard for Kinks in Protein Helices. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2585-2593.	2.5	7
151	Modeling Functional Motions of Biological Systems by Customized Natural Moves. <i>Biophysical Journal</i> , 2016, 111, 710-721.	0.2	7
152	Combining co-evolution and secondary structure prediction to improve fragment library generation. <i>Bioinformatics</i> , 2018, 34, 2219-2227.	1.8	7
153	The Therapeutic Antibody Profiler for Computational Developability Assessment. <i>Methods in Molecular Biology</i> , 2022, 2313, 115-125.	0.4	7
154	Ten simple rules for surviving an interdisciplinary PhD. <i>PLoS Computational Biology</i> , 2017, 13, e1005512.	1.5	7
155	Protein Three-Dimensional Structural Databases: Domains, Structurally Aligned Homologues and Superfamilies. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1998, 54, 1168-1177.	2.5	6
156	A statistical approach using network structure in the prediction of protein characteristics. <i>Bioinformatics</i> , 2007, 23, 2314-2321.	1.8	6
157	Using Phylogeny to Improve Genome-Wide Distant Homology Recognition. <i>PLoS Computational Biology</i> , 2007, 3, e3.	1.5	6
158	pyHVis3D: visualising molecular simulation deduced H-bond networks in 3D: application to T-cell receptor interactions. <i>Bioinformatics</i> , 2018, 34, 1941-1943.	1.8	6
159	COGENT: evaluating the consistency of gene co-expression networks. <i>Bioinformatics</i> , 2021, 37, 1928-1929.	1.8	6
160	Investigating the potential for a limited quantum speedup on protein lattice problems. <i>New Journal of Physics</i> , 0, , .	1.2	6
161	The functional domain grouping of microtubule associated proteins. <i>Communicative and Integrative Biology</i> , 2008, 1, 47-50.	0.6	5
162	Mutual information and variants for protein domain-domain contact prediction. <i>BMC Research Notes</i> , 2012, 5, 472.	0.6	5

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163	Local Network Patterns in Protein-Protein Interfaces. PLoS ONE, 2013, 8, e57031.	1.1	5
164	The evolution of contact prediction: evidence that contact selection in statistical contact prediction is changing. Bioinformatics, 2020, 36, 1750-1756.	1.8	5
165	<i>WONKA</i> and <i>OOMMPPAA</i> : analysis of protein-ligand interaction data to direct structure-based drug design. Acta Crystallographica Section D: Structural Biology, 2017, 73, 279-285.	1.1	5
166	Challenges and Opportunities for Bayesian Statistics in Proteomics. Journal of Proteome Research, 2022, 21, 849-864.	1.8	5
167	<i>In silico</i> structural modeling of multiple epigenetic marks on DNA. Bioinformatics, 2018, 34, 41-48.	1.8	4
168	Ribosome occupancy profiles are conserved between structurally and evolutionarily related yeast domains. Bioinformatics, 2021, 37, 1853-1859.	1.8	4
169	Assessment of model fit via network comparison methods based on subgraph counts. Journal of Complex Networks, 2019, 7, 226-253.	1.1	3
170	RFQAmode: Random Forest Quality Assessment to identify a predicted protein structure in the correct fold. PLoS ONE, 2019, 14, e0218149.	1.1	3
171	High-Throughput Antibody Structure Modeling and Design Using ABodyBuilder. Methods in Molecular Biology, 2019, 1851, 367-380.	0.4	3
172	PROTEIN COMPARATIVE MODELLING AND DRUG DISCOVERY. , 2003, , 445-458.		3
173	A Statistical Model for Helices with Applications. Biometrics, 2018, 74, 845-854.	0.8	2
174	Predicting Inter-Species Cross-Talk in Two-Component Signalling Systems. PLoS ONE, 2012, 7, e37737.	1.1	2
175	Protein Modeling and Structural Prediction. , 2014, , 171-182.		1
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