

# Alexandre Bonvin

## List of Publications by Year in descending order

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281  
papers

25,590  
citations

11639

70  
h-index

9090

144  
g-index

328  
all docs

328  
docs citations

328  
times ranked

24305  
citing authors

#	ARTICLE	IF	CITATIONS
1	HADDOCK: A Protein-Protein Docking Approach Based on Biochemical or Biophysical Information. <i>Journal of the American Chemical Society</i> , 2003, 125, 1731-1737.	6.6	2,642
2	The HADDOCK2.2 Web Server: User-Friendly Integrative Modeling of Biomolecular Complexes. <i>Journal of Molecular Biology</i> , 2016, 428, 720-725.	2.0	2,071
3	The HADDOCK web server for data-driven biomolecular docking. <i>Nature Protocols</i> , 2010, 5, 883-897.	5.5	1,167
4	PRODIGY: a web server for predicting the binding affinity of protein-protein complexes. <i>Bioinformatics</i> , 2016, 32, 3676-3678.	1.8	760
5	Refinement of protein structures in explicit solvent. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 50, 496-506.	1.5	571
6	Structure and Flexibility Adaptation in Nonspecific and Specific Protein-DNA Complexes. <i>Science</i> , 2004, 305, 386-389.	6.0	506
7	The nisin-lipid II complex reveals a pyrophosphate cage that provides a blueprint for novel antibiotics. <i>Nature Structural and Molecular Biology</i> , 2004, 11, 963-967.	3.6	505
8	HADDOCK versus HADDOCK: New features and performance of HADDOCK2.0 on the CAPRI targets. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 69, 726-733.	1.5	504
9	Plectasin, a Fungal Defensin, Targets the Bacterial Cell Wall Precursor Lipid II. <i>Science</i> , 2010, 328, 1168-1172.	6.0	478
10	Sequence co-evolution gives 3D contacts and structures of protein complexes. <i>ELife</i> , 2014, 3, .	2.8	452
11	Contacts-based prediction of binding affinity in protein-protein complexes. <i>ELife</i> , 2015, 4, e07454.	2.8	385
12	Structural Basis for Signal-Sequence Recognition by the Translocase Motor SecA as Determined by NMR. <i>Cell</i> , 2007, 131, 756-769.	13.5	381
13	The $\beta$ -to- $\beta^2$ Conformational Transition of Alzheimer's A $\beta$ (1-42) Peptide in Aqueous Media is Reversible: A Step by Step Conformational Analysis Suggests the Location of $\beta^2$ Conformation Seeding. <i>ChemBioChem</i> , 2006, 7, 257-267.	1.3	375
14	On the binding affinity of macromolecular interactions: daring to ask why proteins interact. <i>Journal of the Royal Society Interface</i> , 2013, 10, 20120835.	1.5	353
15	Updates to the Integrated Protein-Protein Interaction Benchmarks: Docking Benchmark Version 5 and Affinity Benchmark Version 2. <i>Journal of Molecular Biology</i> , 2015, 427, 3031-3041.	2.0	348
16	3D-DART: a DNA structure modelling server. <i>Nucleic Acids Research</i> , 2009, 37, W235-W239.	6.5	330
17	RECOORD: A recalculated coordinate database of 500+ proteins from the PDB using restraints from the BioMagResBank. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 59, 662-672.	1.5	323
18	Structural Biology in the Clouds: The WeNMR-EOSC Ecosystem. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 729513.	1.6	308

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19	Flexible protein-protein docking. <i>Current Opinion in Structural Biology</i> , 2006, 16, 194-200.	2.6	275
20	CPORT: A Consensus Interface Predictor and Its Performance in Prediction-Driven Docking with HADDOCK. <i>PLoS ONE</i> , 2011, 6, e17695.	1.1	272
21	A structure-based benchmark for protein-protein binding affinity. <i>Protein Science</i> , 2011, 20, 482-491.	3.1	252
22	Are Scoring Functions in Protein-Protein Docking Ready To Predict Interactomes? Clues from a Novel Binding Affinity Benchmark. <i>Journal of Proteome Research</i> , 2010, 9, 2216-2225.	1.8	224
23	Short-Chain Fatty Acids Stimulate Angiopoietin-Like 4 Synthesis in Human Colon Adenocarcinoma Cells by Activating Peroxisome Proliferator-Activated Receptor $\beta$ . <i>Molecular and Cellular Biology</i> , 2013, 33, 1303-1316.	1.1	219
24	Assessment of contact predictions in CASP12: Co-evolution and deep learning coming of age. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 51-66.	1.5	174
25	WeNMR: Structural Biology on the Grid. <i>Journal of Grid Computing</i> , 2012, 10, 743-767.	2.5	170
26	Information-driven protein-DNA docking using HADDOCK: it is a matter of flexibility. <i>Nucleic Acids Research</i> , 2006, 34, 3317-3325.	6.5	169
27	A Unified Conformational Selection and Induced Fit Approach to Protein-Peptide Docking. <i>PLoS ONE</i> , 2013, 8, e58769.	1.1	163
28	Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. <i>Processes</i> , 2021, 9, 71.	1.3	162
29	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. <i>Structure</i> , 2015, 23, 1156-1167.	1.6	159
30	Computational prediction of protein interfaces: A review of data driven methods. <i>FEBS Letters</i> , 2015, 589, 3516-3526.	1.3	148
31	Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 323-348.	1.5	148
32	Solvated docking: introducing water into the modelling of biomolecular complexes. <i>Bioinformatics</i> , 2006, 22, 2340-2347.	1.8	143
33	Antimicrobial and Efflux Pump Inhibitory Activity of Caffeoylquinic Acids from <i>Artemisia absinthium</i> against Gram-Positive Pathogenic Bacteria. <i>PLoS ONE</i> , 2011, 6, e18127.	1.1	133
34	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. <i>Journal of Molecular Biology</i> , 2011, 414, 289-302.	2.0	131
35	Large-scale prediction of binding affinity in protein-small ligand complexes: the PRODIGY-LIG web server. <i>Bioinformatics</i> , 2019, 35, 1585-1587.	1.8	130
36	Dynamic binding mode of a Synaptotagmin-1-SNARE complex in solution. <i>Nature Structural and Molecular Biology</i> , 2015, 22, 555-564.	3.6	129

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37	WHISCY: What information does surface conservation yield? Application to data-driven docking. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 63, 479-489.	1.5	128
38	A comprehensive framework of E2â€“RING E3 interactions of the human ubiquitinâ€“proteasome system. <i>Molecular Systems Biology</i> , 2009, 5, 295.	3.2	126
39	Computational approaches to therapeutic antibody design: established methods and emerging trends. <i>Briefings in Bioinformatics</i> , 2020, 21, 1549-1567.	3.2	126
40	Data-driven docking for the study of biomolecular complexes. <i>FEBS Journal</i> , 2005, 272, 293-312.	2.2	125
41	Probing a cell-embedded megadalton protein complex by DNP-supported solid-state NMR. <i>Nature Methods</i> , 2015, 12, 649-652.	9.0	124
42	Conformational Variability of Solution Nuclear Magnetic Resonance Structures. <i>Journal of Molecular Biology</i> , 1995, 250, 80-93.	2.0	123
43	Plasticity in protein-DNA recognition: lac repressor interacts with its natural operator O1 through alternative conformations of its DNA-binding domain. <i>EMBO Journal</i> , 2002, 21, 2866-2876.	3.5	117
44	How Proteins Get in Touch: Interface Prediction in the Study of Biomolecular Complexes. <i>Current Protein and Peptide Science</i> , 2008, 9, 394-406.	0.7	116
45	Building Macromolecular Assemblies by Information-driven Docking. <i>Molecular and Cellular Proteomics</i> , 2010, 9, 1784-1794.	2.5	114
46	NMR Study of Mersacidin and Lipid II Interaction in Dodecylphosphocholine Micelles. <i>Journal of Biological Chemistry</i> , 2003, 278, 13110-13117.	1.6	113
47	Structural Model of the UbcH5B/CNOT4 Complex Revealed by Combining NMR, Mutagenesis, and Docking Approaches. <i>Structure</i> , 2004, 12, 633-644.	1.6	113
48	Data publication with the structural biology data grid supports live analysis. <i>Nature Communications</i> , 2016, 7, 10882.	5.8	113
49	The Solution Structure of the AppA BLUF Domain: Insight into the Mechanism of Light-Induced Signaling. <i>ChemBioChem</i> , 2006, 7, 187-193.	1.3	111
50	NMR analysis of protein interactions. <i>Current Opinion in Chemical Biology</i> , 2005, 9, 501-508.	2.8	109
51	Hydramacin-1, Structure and Antibacterial Activity of a Protein from the Basal Metazoan Hydra. <i>Journal of Biological Chemistry</i> , 2009, 284, 1896-1905.	1.6	107
52	Hydration dynamics of the collagen triple helix by NMR11Edited by P. E. Wright. <i>Journal of Molecular Biology</i> , 2000, 300, 1041-1048.	2.0	103
53	Clustering biomolecular complexes by residue contacts similarity. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 1810-1817.	1.5	103
54	Proteins Feel More Than They See: Fine-Tuning of Binding Affinity by Properties of the Non-Interacting Surface. <i>Journal of Molecular Biology</i> , 2014, 426, 2632-2652.	2.0	103

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55	Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 1200-1221.	1.5	99
56	pdb-tools: a swiss army knife for molecular structures. <i>F1000Research</i> , 2018, 7, 1961.	0.8	99
57	Performance of HADDOCK and a simple contact-based protein-ligand binding affinity predictor in the D3R Grand Challenge 2. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 175-185.	1.3	97
58	Integrative computational modeling of protein interactions. <i>FEBS Journal</i> , 2014, 281, 1988-2003.	2.2	94
59	DRESS: a database of Refined solution NMR structures. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 55, 483-486.	1.5	91
60	Sequence-specific High Mobility Group Box Factors Recognize 10-Base Pair Minor Groove Motifs. <i>Journal of Biological Chemistry</i> , 2000, 275, 27266-27273.	1.6	88
61	Membrane proteins structures: A review on computational modeling tools. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 2021-2039.	1.4	87
62	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 1980-1987.	1.5	87
63	$\beta$ -hairpin stability and folding: molecular dynamics studies of the first $\beta$ -hairpin of tendamistat 1 Edited by A. R. Fersht. <i>Journal of Molecular Biology</i> , 2000, 296, 255-268.	2.0	86
64	Mass Spec Studio for Integrative Structural Biology. <i>Structure</i> , 2014, 22, 1538-1548.	1.6	86
65	Finding the "hot spot": Are predictors of binding affinity changes upon mutations in protein-protein interactions ready for it?. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019, 9, e1410.	6.2	86
66	The solution structure of Lac repressor headpiece 62 complexed to a symmetrical lac operator. <i>Structure</i> , 1999, 7, 1483-53.	1.6	84
67	The Vancomycin-Nisin(1-12) Hybrid Restores Activity against Vancomycin Resistant Enterococci. <i>Biochemistry</i> , 2008, 47, 12661-12663.	1.2	82
68	Water molecules in DNA recognition II: a molecular dynamics view of the structure and hydration of the trp operator 1 Edited by B. Honig. <i>Journal of Molecular Biology</i> , 1998, 282, 859-873.	2.0	80
69	CASD-NMR: critical assessment of automated structure determination by NMR. <i>Nature Methods</i> , 2009, 6, 625-626.	9.0	80
70	Various strategies of using residual dipolar couplings in NMR-driven protein docking: Application to Lys48-linked di-ubiquitin and validation against <sup>15</sup> N-relaxation data. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 60, 367-381.	1.5	78
71	SpotOn: High Accuracy Identification of Protein-Protein Interface Hot-Spots. <i>Scientific Reports</i> , 2017, 7, 8007.	1.6	77
72	Blind Testing of Routine, Fully Automated Determination of Protein Structures from NMR Data. <i>Structure</i> , 2012, 20, 227-236.	1.6	75

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73	â€œEnsembleâ€ iterative relaxation matrix approach: A new NMR refinement protocol applied to the solution structure of crambin. <i>Proteins: Structure, Function and Bioinformatics</i> , 1993, 15, 385-400.	1.5	74
74	The precision of NMR structure ensembles revisited. <i>Journal of Biomolecular NMR</i> , 2003, 25, 225-234.	1.6	74
75	Data-driven docking: HADDOCK's adventures in CAPRI. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 60, 232-238.	1.5	74
76	Structural Determinants of Specific Lipid Binding to Potassium Channels. <i>Journal of the American Chemical Society</i> , 2013, 135, 3983-3988.	6.6	73
77	Prediction of protein assemblies, the next frontier: The <scp>CASP14â€CAPRI</scp> experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 1800-1823.	1.5	73
78	Human galectin-3 (Mac-2 antigen): Defining molecular switches of affinity to natural glycoproteins, structural and dynamic aspects of glycan binding by flexible ligand docking and putative regulatory sequences in the proximal promoter region. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2011, 1810, 150-161.	1.1	72
79	Extended O-GlcNAc on HLA Class-I-Bound Peptides. <i>Journal of the American Chemical Society</i> , 2015, 137, 10922-10925.	6.6	72
80	Do NOE distances contain enough information to assess the relative populations of multi-conformer structures?. <i>Journal of Biomolecular NMR</i> , 1996, 7, 72-6.	1.6	71
81	Detailed Mechanistic Insights into HIV-1 Sensitivity to Three Generations of Fusion Inhibitors. <i>Journal of Biological Chemistry</i> , 2009, 284, 26941-26950.	1.6	71
82	Integrative Modelling of Biomolecular Complexes. <i>Journal of Molecular Biology</i> , 2020, 432, 2861-2881.	2.0	70
83	Nuclear Magnetic Resonance Solution Structure of the Arc Repressor Using Relaxation Matrix Calculations. <i>Journal of Molecular Biology</i> , 1994, 236, 328-341.	2.0	69
84	Integrative Modeling of Biomolecular Complexes: HADDOCKing with Cryo-Electron Microscopy Data. <i>Structure</i> , 2015, 23, 949-960.	1.6	69
85	Mapping the Targeted Membrane Pore Formation Mechanism by Solution NMR:â€ The Nisin Z and Lipid II Interaction in SDS Micelles. <i>Biochemistry</i> , 2002, 41, 7670-7676.	1.2	68
86	Crystal structure and catalytic mechanism of the LPS 3-O-deacylase PagL from <i>Pseudomonas aeruginosa</i> . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 7071-7076.	3.3	68
87	A protein-DNA docking benchmark. <i>Nucleic Acids Research</i> , 2008, 36, e88-e88.	6.5	67
88	Advances in integrative modeling of biomolecular complexes. <i>Methods</i> , 2013, 59, 372-381.	1.9	67
89	dMM-PBSA: A New HADDOCK Scoring Function for Protein-Peptide Docking. <i>Frontiers in Molecular Biosciences</i> , 2016, 3, 46.	1.6	67
90	A Multidomain Flexible Docking Approach to Deal with Large Conformational Changes in the Modeling of Biomolecular Complexes. <i>Structure</i> , 2011, 19, 555-565.	1.6	65

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91	A gp41 MPER-specific Llama VHH Requires a Hydrophobic CDR3 for Neutralization but not for Antigen Recognition. <i>PLoS Pathogens</i> , 2013, 9, e1003202.	2.1	64
92	Refined Structure of lac Repressor Headpiece (1-56) Determined by Relaxation Matrix Calculations from 2D and 3D NOE Data: Change of Tertiary Structure upon Binding to the lac Operator. <i>Journal of Molecular Biology</i> , 1996, 259, 761-773.	2.0	63
93	Defining the limits of homology modeling in information-driven protein docking. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 2119-2128.	1.5	63
94	Sequence-specific HMG box factors recognize 10-12 base pair minor groove motifs. <i>Journal of Biological Chemistry</i> , 2000, 275, 27266-73.	1.6	62
95	Binding Site Structure of One LRP-RAP Complex: Implications for a Common Ligand-Receptor Binding Motif. <i>Journal of Molecular Biology</i> , 2006, 362, 700-716.	2.0	62
96	iScore: a novel graph kernel-based function for scoring protein-protein docking models. <i>Bioinformatics</i> , 2020, 36, 112-121.	1.8	62
97	Insight into cyanobacterial circadian timing from structural details of the KaiB-KaiC interaction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 1379-1384.	3.3	61
98	DisVis: quantifying and visualizing accessible interaction space of distance-restrained biomolecular complexes. <i>Bioinformatics</i> , 2015, 31, 3222-3224.	1.8	61
99	Time- and ensemble-averaged direct NOE restraints. <i>Journal of Biomolecular NMR</i> , 1994, 4, 143-9.	1.6	60
100	NMR Relaxation and Internal Dynamics of Ubiquitin from a 0.2 $\mu$ s MD Simulation. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 363-374.	2.3	60
101	Entropy Calculation of HIV-1 Env gp120, its Receptor CD4, and their Complex: An Analysis of Configurational Entropy Changes upon Complexation. <i>Biophysical Journal</i> , 2005, 88, 15-24.	0.2	60
102	Activity-structure correlations in divergent lectin evolution: fine specificity of chicken galectin CG-14 and computational analysis of flexible ligand docking for CG-14 and the closely related CG-16. <i>Glycobiology</i> , 2007, 17, 165-184.	1.3	60
103	INDIGO-DataCloud: a Platform to Facilitate Seamless Access to E-Infrastructures. <i>Journal of Grid Computing</i> , 2018, 16, 381-408.	2.5	58
104	iSEE: Interface structure, evolution, and energy-based machine learning predictor of binding affinity changes upon mutations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 110-119.	1.5	58
105	Understanding the Role of the Josephin Domain in the PolyUb Binding and Cleavage Properties of Ataxin-3. <i>PLoS ONE</i> , 2010, 5, e12430.	1.1	58
106	Mode of action of teixobactins in cellular membranes. <i>Nature Communications</i> , 2020, 11, 2848.	5.8	57
107	A Docking Approach to the Study of Copper Trafficking Proteins. <i>Structure</i> , 2004, 12, 669-676.	1.6	56
108	Characterization and Structural Analyses of Nonspecific Lipid Transfer Protein 1 from Mung Bean. <i>Biochemistry</i> , 2005, 44, 5703-5712.	1.2	56

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109	Structure of the DNA-bound BRCA1 C-terminal Region from Human Replication Factor C p140 and Model of the Protein-DNA Complex. <i>Journal of Biological Chemistry</i> , 2010, 285, 10087-10097.	1.6	56
110	DeepRank: a deep learning framework for data mining 3D protein-protein interfaces. <i>Nature Communications</i> , 2021, 12, 7068.	5.8	56
111	The solution structure of the human retinoic acid receptor- $\hat{1}^2$ DNA-binding domain. <i>Journal of Biomolecular NMR</i> , 1993, 3, 1-17.	1.6	55
112	On the usefulness of ion-mobility mass spectrometry and SAXS data in scoring docking decoys. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 683-694.	2.5	55
113	Two-rung Model of a Left-handed $\hat{1}^2$ -Helix for Prions Explains Species Barrier and Strain Variation in Transmissible Spongiform Encephalopathies. <i>Journal of Molecular Biology</i> , 2006, 360, 907-920.	2.0	53
114	The orientations of cytochrome c in the highly dynamic complex with cytochrome b5 visualized by NMR and docking using HADDOCK. <i>Protein Science</i> , 2005, 14, 799-811.	3.1	52
115	Pushing the limits of what is achievable in protein-DNA docking: benchmarking HADDOCK's performance. <i>Nucleic Acids Research</i> , 2010, 38, 5634-5647.	6.5	51
116	Modeling Protein-Protein Complexes Using the HADDOCK Webserver - Modeling Protein Complexes with HADDOCK. <i>Methods in Molecular Biology</i> , 2014, 1137, 163-179.	0.4	51
117	Modeling Antibody-Antigen Complexes by Information-Driven Docking. <i>Structure</i> , 2020, 28, 119-129.e2.	1.6	51
118	Emergence and spread of SARS-CoV-2 lineage B.1.620 with variant of concern-like mutations and deletions. <i>Nature Communications</i> , 2021, 12, 5769.	5.8	51
119	BioMagResBank databases DOCR and FRED containing converted and filtered sets of experimental NMR restraints and coordinates from over 500 protein PDB structures. <i>Journal of Biomolecular NMR</i> , 2005, 32, 1-12.	1.6	50
120	Turning Defense into Offense: Defensin Mimetics as Novel Antibiotics Targeting Lipid II. <i>PLoS Pathogens</i> , 2013, 9, e1003732.	2.1	50
121	Blind prediction of interfacial water positions in CAPRI. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 620-632.	1.5	50
122	The Supramolecular Organization of a Peptide-Based Nanocarrier at High Molecular Detail. <i>Journal of the American Chemical Society</i> , 2015, 137, 7775-7784.	6.6	50
123	Fast and sensitive rigid-body fitting into cryo-EM density maps with PowerFit. <i>AIMS Biophysics</i> , 2015, 2, 73-87.	0.3	49
124	Model for RNA Binding and the Catalytic Site of the RNase Kid of the Bacterial parD Toxin-Antitoxin System. <i>Journal of Molecular Biology</i> , 2006, 357, 115-126.	2.0	48
125	Importance of lipid-pore loop interface for potassium channel structure and function. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 13008-13013.	3.3	48
126	Water molecules in DNA recognition I: hydration lifetimes of trp operator DNA in solution measured by NMR spectroscopy 1 Edited by B. Honig. <i>Journal of Molecular Biology</i> , 1998, 282, 847-858.	2.0	47



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127	Gentamicin Binds to the Megalin Receptor as a Competitive Inhibitor Using the Common Ligand Binding Motif of Complement Type Repeats. <i>Journal of Biological Chemistry</i> , 2013, 288, 4424-4435.	1.6	47
128	Solution structure and DNA-binding properties of the C-terminal domain of UvrC from E.coli. <i>EMBO Journal</i> , 2002, 21, 6257-6266.	3.5	46
129	Active-site architecture and catalytic mechanism of the lipid A deacylase LpxR of <i>Salmonella typhimurium</i> . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 1960-1964.	3.3	46
130	Specificity and Affinity of Lac Repressor for the Auxiliary Operators O2 and O3 Are Explained by the Structures of Their Protein-DNA Complexes. <i>Journal of Molecular Biology</i> , 2009, 390, 478-489.	2.0	46
131	Protein-protein HADDOCKing using exclusively pseudocontact shifts. <i>Journal of Biomolecular NMR</i> , 2011, 50, 263-266.	1.6	46
132	A Machine Learning Approach for Hot-Spot Detection at Protein-Protein Interfaces. <i>International Journal of Molecular Sciences</i> , 2016, 17, 1215.	1.8	46
133	PRODIGY: A Contact-based Predictor of Binding Affinity in Protein-protein Complexes. <i>Bio-protocol</i> , 2017, 7, e2124.	0.2	46
134	Kinetics and Thermodynamics of Type VIII $\beta$ -Turn Formation: A CD, NMR, and Microsecond Explicit Molecular Dynamics Study of the GDNP Tetrapeptide. <i>Biophysical Journal</i> , 2006, 90, 2745-2759.	0.2	44
135	Sense and simplicity in <i>HADDOCK</i> scoring: Lessons from <i>CASP-CAPRI</i> round 1. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 417-423.	1.5	44
136	The DisVis and PowerFit Web Servers: Explorative and Integrative Modeling of Biomolecular Complexes. <i>Journal of Molecular Biology</i> , 2017, 429, 399-407.	2.0	43
137	Less Is More: Coarse-Grained Integrative Modeling of Large Biomolecular Assemblies with HADDOCK. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6358-6367.	2.3	43
138	Impaired Peroxisome Proliferator-Activated Receptor $\beta$ Function through Mutation of a Conserved Salt Bridge (R425C) in Familial Partial Lipodystrophy. <i>Molecular Endocrinology</i> , 2007, 21, 1049-1065.	3.7	42
139	Direct NOE refinement of biomolecular structures using 2D NMR data. <i>Journal of Biomolecular NMR</i> , 1991, 1, 305-309.	1.6	41
140	Atomic insight into the CD4 binding-induced conformational changes in HIV-1 gp120. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 55, 582-593.	1.5	39
141	Combining NMR Relaxation with Chemical Shift Perturbation Data to Drive Protein-protein Docking. <i>Journal of Biomolecular NMR</i> , 2006, 34, 237-244.	1.6	39
142	M3: an integrative framework for structure determination of molecular machines. <i>Nature Methods</i> , 2017, 14, 897-902.	9.0	39
143	Inhibition of the integrated stress response by viral proteins that block p-eIF2-eIF2B association. <i>Nature Microbiology</i> , 2020, 5, 1361-1373.	5.9	39
144	Immunogenicity of Peptide-vaccine Candidates Predicted by Molecular Dynamics Simulations. <i>Journal of Molecular Biology</i> , 2003, 328, 1083-1089.	2.0	37

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145	Data-driven homology modelling of a glycoprotein in the ATP-bound state indicates flexibility of the transmembrane domains. <i>FEBS Journal</i> , 2009, 276, 964-972.	2.2	37
146	Characterizing the N- and C-terminal Small Ubiquitin-like Modifier (SUMO)-interacting Motifs of the Scaffold Protein DAXX. <i>Journal of Biological Chemistry</i> , 2011, 286, 19816-19829.	1.6	37
147	Molecular origins of binding affinity: seeking the Archimedean point. <i>Current Opinion in Structural Biology</i> , 2013, 23, 868-877.	2.6	37
148	Strengths and weaknesses of data-driven docking in critical assessment of prediction of interactions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 3242-3249.	1.5	36
149	Rapid prediction of multi-dimensional NMR data sets. <i>Journal of Biomolecular NMR</i> , 2012, 54, 377-387.	1.6	35
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