Alexandre Bonvin

List of Publications by Year
in descending order

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281 papers	25,590 citations	11608 70 h-index	9073 144 g-index
328 all docs	328 docs citations	328 times ranked	24305 citing authors

#	Article	IF	Citations
1	HADDOCK:Â A Proteinâ"Protein Docking Approach Based on Biochemical or Biophysical Information. Journal of the American Chemical Society, 2003, 125, 1731-1737.	6.6	2,642
2	The HADDOCK2.2 Web Server: User-Friendly Integrative Modeling of Biomolecular Complexes. Journal of Molecular Biology, 2016, 428, 720-725.	2.0	2,071
3	The HADDOCK web server for data-driven biomolecular docking. Nature Protocols, 2010, 5, 883-897.	5.5	1,167
4	PRODIGY: a web server for predicting the binding affinity of proteinâ€"protein complexes. Bioinformatics, 2016, 32, 3676-3678.	1.8	760
5	Refinement of protein structures in explicit solvent. Proteins: Structure, Function and Bioinformatics, 2003, 50, 496-506.	1.5	571
6	Structure and Flexibility Adaptation in Nonspecific and Specific Protein-DNA Complexes. Science, 2004, 305, 386-389.	6.0	506
7	The nisinâ€"lipid II complex reveals a pyrophosphate cage that provides a blueprint for novel antibiotics. Nature Structural and Molecular Biology, 2004, 11, 963-967.	3.6	505
8	HADDOCK versus HADDOCK: New features and performance of HADDOCK2.0 on the CAPRI targets. Proteins: Structure, Function and Bioinformatics, 2007, 69, 726-733.	1.5	504
9	Plectasin, a Fungal Defensin, Targets the Bacterial Cell Wall Precursor Lipid II. Science, 2010, 328, 1168-1172.	6.0	478
10	Sequence co-evolution gives 3D contacts and structures of protein complexes. ELife, 2014, 3, .	2.8	452
11	Contacts-based prediction of binding affinity in proteinâ€"protein complexes. ELife, 2015, 4, e07454.	2.8	385
12	Structural Basis for Signal-Sequence Recognition by the Translocase Motor SecA as Determined by NMR. Cell, 2007, 131, 756-769.	13.5	381
13	The Î±-to-Î² Conformational Transition of Alzheimer's AÎ²-(1-42) Peptide in Aqueous Media is Reversible: A Step by Step Conformational Analysis Suggests the Location of Î² Conformation Seeding. ChemBioChem, 2006, 7, 257-267.	1.3	375
14	On the binding affinity of macromolecular interactions: daring to ask why proteins interact. Journal of the Royal Society Interface, 2013, 10, 20120835.	1.5	353
15	Updates to the Integrated Proteinâ€"Protein Interaction Benchmarks: Docking Benchmark Version 5 and Affinity Benchmark Version 2. Journal of Molecular Biology, 2015, 427, 3031-3041.	2.0	348
16	3D-DART: a DNA structure modelling server. Nucleic Acids Research, 2009, 37, W235-W239.	6.5	330
17	RECOORD: A recalculated coordinate database of 500+ proteins from the PDB using restraints from the BioMagResBank. Proteins: Structure, Function and Bioinformatics, 2005, 59, 662-672.	1.5	323
18	Structural Biology in the Clouds: The WeNMR-EOSC Ecosystem. Frontiers in Molecular Biosciences, 2021, 8, 729513.	1.6	308

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19	Flexible proteinâ€“protein docking. Current Opinion in Structural Biology, 2006, 16, 194-200.	2.6	275
20	CPORT: A Consensus Interface Predictor and Its Performance in Prediction-Driven Docking with HADDOCK. PLoS ONE, 2011, 6, e17695.	1.1	272
21	A structureâ€based benchmark for proteinâ€“protein binding affinity. Protein Science, 2011, 20, 482-491.	3.1	252
22	Are Scoring Functions in Proteinâ^'Protein Docking Ready To Predict Interactomes? Clues from a Novel Binding Affinity Benchmark. Journal of Proteome Research, 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 Î³. Molecular and Cellular Biology, 2013, 33, 1303-1316.	1.1	219
24	Assessment of contact predictions in CASP12: Coâ€evolution and deep learning coming of age. Proteins: Structure, Function and Bioinformatics, 2018, 86, 51-66.	1.5	174
25	WeNMR: Structural Biology on the Grid. Journal of Grid Computing, 2012, 10, 743-767.	2.5	170
26	Information-driven protein-DNA docking using HADDOCK: it is a matter of flexibility. Nucleic Acids Research, 2006, 34, 3317-3325.	6.5	169
27	A Unified Conformational Selection and Induced Fit Approach to Protein-Peptide Docking. PLoS ONE, 2013, 8, e58769.	1.1	163
28	Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. Processes, 2021, 9, 71.	1.3	162
29	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. Structure, 2015, 23, 1156-1167.	1.6	159
30	Computational prediction of protein interfaces: A review of data driven methods. FEBS Letters, 2015, 589, 3516-3526.	1.3	148
31	Prediction of homoprotein and heteroprotein complexes by protein docking and templateâ€based modeling: A CASPâ€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2016, 84, 323-348.	1.5	148
32	Solvated docking: introducing water into the modelling of biomolecular complexes. Bioinformatics, 2006, 22, 2340-2347.	1.8	143
33	Antimicrobial and Efflux Pump Inhibitory Activity of Caffeoylquinic Acids from Artemisia absinthium against Gram-Positive Pathogenic Bacteria. PLoS ONE, 2011, 6, e18127.	1.1	133
34	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	2.0	131
35	Large-scale prediction of binding affinity in proteinâ€“small ligand complexes: the PRODIGY-LIG web server. Bioinformatics, 2019, 35, 1585-1587.	1.8	130
36	Dynamic binding mode of a Synaptotagmin-1â€“SNARE complex in solution. Nature Structural and Molecular Biology, 2015, 22, 555-564.	3.6	129

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

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55	Blind prediction of homoâ€•and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	1.5	99
56	pdb-tools: a swiss army knife for molecular structures. F1000Research, 2018, 7, 1961.	0.8	99
57	Performance of HADDOCK and a simple contact-based proteinâ€“ligand binding affinity predictor in the D3R Grand Challenge 2. Journal of Computer-Aided Molecular Design, 2018, 32, 175-185.	1.3	97
58	Integrative computational modeling of protein interactions. FEBS Journal, 2014, 281, 1988-2003.	2.2	94
59	DRESS: a database of REfined solution NMR structures. Proteins: Structure, Function and Bioinformatics, 2004, 55, 483-486.	1.5	91
60	Sequence-specific High Mobility Group Box Factors Recognize 10â€“12-Base Pair Minor Groove Motifs. Journal of Biological Chemistry, 2000, 275, 27266-27273.	1.6	88
61	Membrane proteins structures: A review on computational modeling tools. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 2021-2039.	1.4	87
62	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1980-1987.	1.5	87
63	Î²-hairpin stability and folding: molecular dynamics studies of the first Î²-hairpin of tendamistat 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 2000, 296, 255-268.	2.0	86
64	Mass Spec Studio for Integrative Structural Biology. Structure, 2014, 22, 1538-1548.	1.6	86
65	Finding the Î”Î”‹i›G‹/i› spot: Are predictors of binding affinity changes upon mutations in proteinâ€“protein interactions ready for it?. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1410.	6.2	86
66	The solution structure of Lac repressor headpiece 62 complexed to a symmetrical lac operator. Structure, 1999, 7, 1483-S3.	1.6	84
67	The Vancomycinâ^'Nisin(1â^'12) Hybrid Restores Activity against Vancomycin Resistant Enterococci. Biochemistry, 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 1Edited by B. Honig. Journal of Molecular Biology, 1998, 282, 859-873.	2.0	80
69	CASD-NMR: critical assessment of automated structure determination by NMR. Nature Methods, 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 15N-relaxation data. Proteins: Structure, Function and Bioinformatics, 2005, 60, 367-381.	1.5	78
71	SpotOn: High Accuracy Identification of Protein-Protein Interface Hot-Spots. Scientific Reports, 2017, 7, 8007.	1.6	77
72	Blind Testing of Routine, Fully Automated Determination of Protein Structures from NMR Data. Structure, 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. Proteins: Structure, Function and Bioinformatics, 1993, 15, 385-400.	1.5	74
74	The precision of NMR structure ensembles revisited. Journal of Biomolecular NMR, 2003, 25, 225-234.	1.6	74
75	Data-driven docking: HADDOCK's adventures in CAPRI. Proteins: Structure, Function and Bioinformatics, 2005, 60, 232-238.	1.5	74
76	Structural Determinants of Specific Lipid Binding to Potassium Channels. Journal of the American Chemical Society, 2013, 135, 3983-3988.	6.6	73
77	Prediction of protein assemblies, the next frontier: The <scp>CASP14â€CAPRI</scp> experiment. Proteins: Structure, Function and Bioinformatics, 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. Biochimica Et Biophysica Acta - General Subjects, 2011, 1810, 150-161.	1.1	72
79	Extended O-GlcNAc on HLA Class-I-Bound Peptides. Journal of the American Chemical Society, 2015, 137, 10922-10925.	6.6	72
80	Do NOE distances contain enough information to assess the relative populations of multi-conformer structures?. Journal of Biomolecular NMR, 1996, 7, 72-6.	1.6	71
81	Detailed Mechanistic Insights into HIV-1 Sensitivity to Three Generations of Fusion Inhibitors. Journal of Biological Chemistry, 2009, 284, 26941-26950.	1.6	71
82	Integrative Modelling of Biomolecular Complexes. Journal of Molecular Biology, 2020, 432, 2861-2881.	2.0	70
83	Nuclear Magnetic Resonance Solution Structure of the Arc Repressor Using Relaxation Matrix Calculations. Journal of Molecular Biology, 1994, 236, 328-341.	2.0	69
84	Integrative Modeling of Biomolecular Complexes: HADDOCKing with Cryo-Electron Microscopy Data. Structure, 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. Biochemistry, 2002, 41, 7670-7676.	1.2	68
86	Crystal structure and catalytic mechanism of the LPS 3-O-deacylase PagL from Pseudomonas aeruginosa. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 7071-7076.	3.3	68
87	A protein-DNA docking benchmark. Nucleic Acids Research, 2008, 36, e88-e88.	6.5	67
88	Advances in integrative modeling of biomolecular complexes. Methods, 2013, 59, 372-381.	1.9	67
89	dMM-PBSA: A New HADDOCK Scoring Function for Protein-Peptide Docking. Frontiers in Molecular Biosciences, 2016, 3, 46.	1.6	67
90	A Multidomain Flexible Docking Approach to Deal with Large Conformational Changes in the Modeling of Biomolecular Complexes. Structure, 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. PLoS Pathogens, 2013, 9, e1003202.	2.1	64
92	Refined Structure oflacRepressor Headpiece (1-56) Determined by Relaxation Matrix Calculations from 2D and 3D NOE Data: Change of Tertiary Structure upon Binding to thelacOperator. Journal of Molecular Biology, 1996, 259, 761-773.	2.0	63
93	Defining the limits of homology modeling in informationâ€driven protein docking. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2119-2128.	1.5	63
94	Sequence-specific HMG box factors recognize 10-12 base pair minor groove motifs. Journal of Biological Chemistry, 2000, 275, 27266-73.	1.6	62
95	Binding Site Structure of One LRPâ€“RAP Complex:Implications for a Common Ligandâ€“Receptor Binding Motif. Journal of Molecular Biology, 2006, 362, 700-716.	2.0	62
96	iScore: a novel graph kernel-based function for scoring proteinâ€“protein docking models. Bioinformatics, 2020, 36, 112-121.	1.8	62
97	Insight into cyanobacterial circadian timing from structural details of the KaiBâ€“KaiC interaction. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 1379-1384.	3.3	61
98	DisVis: quantifying and visualizing accessible interaction space of distance-restrained biomolecular complexes. Bioinformatics, 2015, 31, 3222-3224.	1.8	61
99	Time- and ensemble-averaged direct NOE restraints. Journal of Biomolecular NMR, 1994, 4, 143-9.	1.6	60
100	NMR Relaxation and Internal Dynamics of Ubiquitin from a 0.2 Î¼s MD Simulation. Journal of Chemical Theory and Computation, 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. Biophysical Journal, 2005, 88, 15-24.	0.2	60
102	Activityâ€“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. Glycobiology, 2007, 17, 165-184.	1.3	60
103	INDIGO-DataCloud: a Platform to Facilitate Seamless Access to E-Infrastructures. Journal of Grid Computing, 2018, 16, 381-408.	2.5	58
104	iSEE: Interface structure, evolution, and energyâ€based machine learning predictor of binding affinity changes upon mutations. Proteins: Structure, Function and Bioinformatics, 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. PLoS ONE, 2010, 5, e12430.	1.1	58
106	Mode of action of teixobactins in cellular membranes. Nature Communications, 2020, 11, 2848.	5.8	57
107	A Docking Approach to the Study of Copper Trafficking Proteins. Structure, 2004, 12, 669-676.	1.6	56
108	Characterization and Structural Analyses of Nonspecific Lipid Transfer Protein 1 from Mung Beanâ€,â€¡. Biochemistry, 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. Journal of Biological Chemistry, 2010, 285, 10087-10097.	1.6	56
110	DeepRank: a deep learning framework for data mining 3D protein-protein interfaces. Nature Communications, 2021, 12, 7068.	5.8	56
111	The solution structure of the human retinoic acid receptor-Î² DNA-binding domain. Journal of Biomolecular NMR, 1993, 3, 1-17.	1.6	55
112	On the usefulness of ion-mobility mass spectrometry and SAXS data in scoring docking decoys. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 683-694.	2.5	55
113	Two-rung Model of a Left-handed Î²-Helix for Prions Explains Species Barrier and Strain Variation in Transmissible Spongiform Encephalopathies. Journal of Molecular Biology, 2006, 360, 907-920.	2.0	53
114	The orientations of cytochromecin the highly dynamic complex with cytochromeb5visualized by NMR and docking using HADDOCK. Protein Science, 2005, 14, 799-811.	3.1	52
115	Pushing the limits of what is achievable in proteinâ€“DNA docking: benchmarking HADDOCKâ€™s performance. Nucleic Acids Research, 2010, 38, 5634-5647.	6.5	51
116	Modeling Proteinâ€“Protein Complexes Using the HADDOCK Webserver â€œModeling Protein Complexes with HADDOCKâ€• Methods in Molecular Biology, 2014, 1137, 163-179.	0.4	51
117	Modeling Antibody-Antigen Complexes by Information-Driven Docking. Structure, 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. Nature Communications, 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. Journal of Biomolecular NMR, 2005, 32, 1-12.	1.6	50
120	Turning Defense into Offense: Defensin Mimetics as Novel Antibiotics Targeting Lipid II. PLoS Pathogens, 2013, 9, e1003732.	2.1	50
121	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	1.5	50
122	The Supramolecular Organization of a Peptide-Based Nanocarrier at High Molecular Detail. Journal of the American Chemical Society, 2015, 137, 7775-7784.	6.6	50
123	Fast and sensitive rigid-body fitting into cryo-EM density maps with PowerFit. AIMS Biophysics, 2015, 2, 73-87.	0.3	49
124	Model for RNA Binding and the Catalytic Site of the RNase Kid of the Bacterial parD Toxinâ€“Antitoxin System. Journal of Molecular Biology, 2006, 357, 115-126.	2.0	48
125	Importance of lipidâ€“pore loop interface for potassium channel structure and function. Proceedings of the National Academy of Sciences of the United States of America, 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 1Edited by B. Honig. Journal of Molecular Biology, 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. Journal of Biological Chemistry, 2013, 288, 4424-4435.	1.6	47
128	Solution structure and DNA-binding properties of the C-terminal domain of UvrC from E.coli. EMBO Journal, 2002, 21, 6257-6266.	3.5	46
129	Active-site architecture and catalytic mechanism of the lipid A deacylase LpxR of Salmonella typhimurium. Proceedings of the National Academy of Sciences of the United States of America, 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 Proteinâ€“DNA Complexes. Journal of Molecular Biology, 2009, 390, 478-489.	2.0	46
131	Proteinâ€“protein HADDocking using exclusively pseudocontact shifts. Journal of Biomolecular NMR, 2011, 50, 263-266.	1.6	46
132	A Machine Learning Approach for Hot-Spot Detection at Protein-Protein Interfaces. International Journal of Molecular Sciences, 2016, 17, 1215.	1.8	46
133	PRODIGY: A Contact-based Predictor of Binding Affinity in Protein-protein Complexes. Bio-protocol, 2017, 7, e2124.	0.2	46
134	Kinetics and Thermodynamics of Type VIII Î²-Turn Formation: A CD, NMR, and Microsecond Explicit Molecular Dynamics Study of the GDNP Tetrapeptide. Biophysical Journal, 2006, 90, 2745-2759.	0.2	44
135	Sense and simplicity in <scp>HADDOCK</scp> scoring: Lessons from <scp>CASPâ€CAPRI</scp> round 1. Proteins: Structure, Function and Bioinformatics, 2017, 85, 417-423.	1.5	44
136	The DisVis and PowerFit Web Servers: Explorative and Integrative Modeling of Biomolecular Complexes. Journal of Molecular Biology, 2017, 429, 399-407.	2.0	43
137	Less Is More: Coarse-Grained Integrative Modeling of Large Biomolecular Assemblies with HADDOCK. Journal of Chemical Theory and Computation, 2019, 15, 6358-6367.	2.3	43
138	Impaired Peroxisome Proliferator-Activated Receptor Î³ Function through Mutation of a Conserved Salt Bridge (R425C) in Familial Partial Lipodystrophy. Molecular Endocrinology, 2007, 21, 1049-1065.	3.7	42
139	Direct NOE refinement of biomolecular structures using 2D NMR data. Journal of Biomolecular NMR, 1991, 1, 305-309.	1.6	41
140	Atomic insight into the CD4 binding-induced conformational changes in HIV-1 gp120. Proteins: Structure, Function and Bioinformatics, 2004, 55, 582-593.	1.5	39
141	Combining NMR Relaxation with Chemical Shift Perturbation Data to Drive Proteinâ€“protein Docking. Journal of Biomolecular NMR, 2006, 34, 237-244.	1.6	39
142	M3: an integrative framework for structure determination of molecular machines. Nature Methods, 2017, 14, 897-902.	9.0	39
143	Inhibition of the integrated stress response by viral proteins that block p-eIF2â€“eIF2B association. Nature Microbiology, 2020, 5, 1361-1373.	5.9	39
144	Immunogenicity of Peptide-vaccine Candidates Predicted by Molecular Dynamics Simulations. Journal of Molecular Biology, 2003, 328, 1083-1089.	2.0	37

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145	Dataâ€driven homology modelling of Pâ€glycoprotein in the ATPâ€bound state indicates flexibility of the transmembrane domains. FEBS Journal, 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. Journal of Biological Chemistry, 2011, 286, 19816-19829.	1.6	37
147	Molecular origins of binding affinity: seeking the Archimedean point. Current Opinion in Structural Biology, 2013, 23, 868-877.	2.6	37
148	Strengths and weaknesses of dataâ€driven docking in critical assessment of prediction of interactions. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3242-3249.	1.5	36
149	Rapid prediction of multi-dimensional NMR data sets. Journal of Biomolecular NMR, 2012, 54, 377-387.	1.6	35
150	Information-Driven, Ensemble Flexible Peptide Docking Using HADDOCK. Methods in Molecular Biology, 2017, 1561, 109-138.	0.4	35
151	On the molecular basis of the recognition of angiotensin II (AII). FEBS Journal, 2003, 270, 849-860.	0.2	33
152	Holo-like and Druggable Protein Conformations from Enhanced Sampling of Binding Pocket Volume and Shape. Journal of Chemical Information and Modeling, 2019, 59, 1515-1528.	2.5	33
153	A Flexible, Grid-Enabled Web Portal for GROMACS Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3463-3472.	2.3	32
154	Preâ€and postâ€docking sampling of conformational changes using ClustENM and HADDOCK for proteinâ€protein and proteinâ€DNA systems. Proteins: Structure, Function and Bioinformatics, 2020, 88, 292-306.	1.5	32
155	The GROMOS96 benchmarks for molecular simulation. Computer Physics Communications, 2000, 128, 550-557.	3.0	31
156	Solution Structure of the Ubiquitin-conjugating Enzyme UbcH5B. Journal of Molecular Biology, 2004, 344, 513-526.	2.0	31
157	Integrative modeling of membrane-associated protein assemblies. Nature Communications, 2020, 11, 6210.	5.8	31
158	Toward an NMR R factor. Journal of Magnetic Resonance, 1991, 91, 659-664.	0.5	30
159	HADDOCK_{2P2I}: A Biophysical Model for Predicting the Binding Affinity of Proteinâ€“Protein Interaction Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 826-836.	2.5	30
160	LightDock goes information-driven. Bioinformatics, 2020, 36, 950-952.	1.8	30
161	Information-driven modeling of large macromolecular assemblies using NMR data. Journal of Magnetic Resonance, 2014, 241, 103-114.	1.2	29
162	A benchmark testing ground for integrating homology modeling and protein docking. Proteins: Structure, Function and Bioinformatics, 2017, 85, 10-16.	1.5	29

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163	Localisation and dynamics of sodium counterions around DNA in solution from molecular dynamics simulation. European Biophysics Journal, 2000, 29, 57-60.	1.2	28
164	Supramolecular Organization and Functional Implications of K⁺â€...Channel Clusters in Membranes. Angewandte Chemie - International Edition, 2017, 56, 13222-13227.	7.2	28
165	MARTINI-Based Protein-DNA Coarse-Grained HADDOCKing. Frontiers in Molecular Biosciences, 2019, 6, 102.	1.6	28
166	Modeling Proteinâ^'Protein Complexes Involved in the CytochromecOxidase Copper-Delivery Pathway. Journal of Proteome Research, 2007, 6, 1530-1539.	1.8	27
167	NMRâ€based modeling and binding studies of a ternary complex between chicken liver bile acid binding protein and bile acids. Proteins: Structure, Function and Bioinformatics, 2007, 69, 177-191.	1.5	27
168	proABC-2: PRediction of AntiBody contacts v2 and its application to information-driven docking. Bioinformatics, 2020, 36, 5107-5108.	1.8	27
169	Next challenges in proteinâ€“protein docking: from proteome to interactome and beyond. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 642-651.	6.2	26
170	Solvated proteinâ€“protein docking using Kyteâ€Doolittleâ€based water preferences. Proteins: Structure, Function and Bioinformatics, 2013, 81, 510-518.	1.5	26
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