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	Using machineâ€learningâ€driven approaches to boost hotâ€spot's knowledge. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	2
2	Molecular Insights Into Binding and Activation of the Human KCNQ2 Channel by Retigabine. Frontiers in Molecular Biosciences, 2022, 9, 839249.	1.6	1
3	Interface refinement of low- to medium-resolution Cryo-EM complexes using HADDOCK2.4. Structure, 2022, 30, 476-484.e3.	1.6	5
4	Cyclization and Docking Protocol for Cyclic Peptideâ€“Protein Modeling Using HADDOCK2.4. Journal of Chemical Theory and Computation, 2022, 18, 4027-4040.	2.3	12
5	Pathogen-sugar interactions revealed by universal saturation transfer analysis. Science, 2022, 377, .	6.0	24
6	<scp>PDBâ€tools</scp> web: A userâ€friendly interface for the manipulation of <scp>PDB</scp> files. Proteins: Structure, Function and Bioinformatics, 2021, 89, 330-335.	1.5	15
7	Integrating quantitative proteomics with accurate genome profiling of transcription factors by greenCUT&RUN. Nucleic Acids Research, 2021, 49, e49.	6.5	14
8	Characterization of nucleosome sediments for protein interaction studies by solid-state NMR spectroscopy. Magnetic Resonance, 2021, 2, 187-202.	0.8	9
9	50 years of PDB: a catalyst in structural biology. Nature Methods, 2021, 18, 448-449.	9.0	12
10	Structural Biology in the Clouds: The WeNMR-EOSC Ecosystem. Frontiers in Molecular Biosciences, 2021, 8, 729513.	1.6	308
11	Shape-Restrained Modeling of Proteinâ€“Small-Molecule Complexes with High Ambiguity Driven DOCKing. Journal of Chemical Information and Modeling, 2021, 61, 4807-4818.	2.5	11
12	Native or Non-Native Proteinâ€“Protein Docking Models? Molecular Dynamics to the Rescue. Journal of Chemical Theory and Computation, 2021, 17, 5944-5954.	2.3	21
13	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
14	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
15	Information-driven modeling of biomolecular complexes. Current Opinion in Structural Biology, 2021, 70, 70-77.	2.6	11
16	MENSAdb: a thorough structural analysis of membrane protein dimers. Database: the Journal of Biological Databases and Curation, 2021, 2021, .	1.4	2
17	Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. Processes, 2021, 9, 71.	1.3	162
18	DeepRank: a deep learning framework for data mining 3D protein-protein interfaces. Nature Communications, 2021, 12, 7068.	5.8	56

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19	iScore: a novel graph kernel-based function for scoring proteinâ€“protein docking models. Bioinformatics, 2020, 36, 112-121.	1.8	62
20	Computational approaches to therapeutic antibody design: established methods and emerging trends. Briefings in Bioinformatics, 2020, 21, 1549-1567.	3.2	126
21	LightDock goes information-driven. Bioinformatics, 2020, 36, 950-952.	1.8	30
22	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
23	The structural details of the interaction of singleâ€stranded DNA binding protein hSSB2 (NABP1/OBFC2A) with UVâ€damaged DNA. Proteins: Structure, Function and Bioinformatics, 2020, 88, 319-326.	1.5	10
24	Coupling enhanced sampling of the apo-receptor with template-based ligand conformers selection: performance in pose prediction in the D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2020, 34, 149-162.	1.3	11
25	An overview of dataâ€driven HADDOCK strategies in CAPRI rounds 38â€45. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1029-1036.	1.5	11
26	Modeling Antibody-Antigen Complexes by Information-Driven Docking. Structure, 2020, 28, 119-129.e2.	1.6	51
27	Integrative Modelling of Biomolecular Complexes. Journal of Molecular Biology, 2020, 432, 2861-2881.	2.0	70
28	Inhibition of the integrated stress response by viral proteins that block p-eIF2â€“eIF2B association. Nature Microbiology, 2020, 5, 1361-1373.	5.9	39
29	Editorial: Multiscale Modeling From Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations. Frontiers in Molecular Biosciences, 2020, 7, 194.	1.6	8
30	Integrative modeling of membrane-associated protein assemblies. Nature Communications, 2020, 11, 6210.	5.8	31
31	Control over the fibrillization yield by varying the oligomeric nucleation propensities of self-assembling peptides. Communications Chemistry, 2020, 3, .	2.0	7
32	proABC-2: PRediction of AntiBody contacts v2 and its application to information-driven docking. Bioinformatics, 2020, 36, 5107-5108.	1.8	27
33	Coarse-grained (hybrid) integrative modeling of biomolecular interactions. Computational and Structural Biotechnology Journal, 2020, 18, 1182-1190.	1.9	23
34	Mode of action of teixobactins in cellular membranes. Nature Communications, 2020, 11, 2848.	5.8	57
35	Biological vs. Crystallographic Protein Interfaces: An Overview of Computational Approaches for Their Classification. Crystals, 2020, 10, 114.	1.0	15
36	EDES: A Protocol to Generate Holo-Like and Druggable Protein Conformations Starting from the APO Structure. Biophysical Journal, 2020, 118, 44a.	0.2	0

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37	Proteinâ€“Protein Modeling Using Cryo-EM Restraints. Methods in Molecular Biology, 2020, 2112, 145-162.	0.4	3
38	iScore: An MPI supported software for ranking proteinâ€“protein docking models based on a random walk graph kernel and support vector machines. SoftwareX, 2020, 11, 100462.	1.2	5
39	A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf	6.8	12
40	Understanding Docking Complexes of Macromolecules Using HADDOCK: The Synergy between Experimental Data and Computations. Bio-protocol, 2020, 10, e3793.	0.2	6
41	A click-flipped enzyme substrate boosts the performance of the diagnostic screening for Hunter syndrome. Chemical Science, 2020, 11, 12671-12676.	3.7	1
42	Blind prediction of homoâ€•and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	1.5	99
43	MARTINI-Based Protein-DNA Coarse-Grained HADDOCKing. Frontiers in Molecular Biosciences, 2019, 6, 102.	1.6	28
44	Sharing Data from Molecular Simulations. Journal of Chemical Information and Modeling, 2019, 59, 4093-4099.	2.5	26
45	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
46	Folding Then Binding vs Folding Through Binding in Macrocyclic Peptide Inhibitors of Human Pancreatic Î±-Amylase. ACS Chemical Biology, 2019, 14, 1751-1759.	1.6	16
47	PRODIGY-crystal: a web-tool for classification of biological interfaces in protein complexes. Bioinformatics, 2019, 35, 4821-4823.	1.8	26
48	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
49	West-Life: A Virtual Research Environment for structural biology. Journal of Structural Biology: X, 2019, 1, 100006.	0.7	2
50	Large-scale prediction of binding affinity in proteinâ€“small ligand complexes: the PRODIGY-LIG web server. Bioinformatics, 2019, 35, 1585-1587.	1.8	130
51	Natural helix 9 mutants of PPARÎ³ differently affect its transcriptional activity. Molecular Metabolism, 2019, 20, 115-127.	3.0	12
52	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
53	Finding the Î”Î”G 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
54	Proteinâ€“ligand pose and affinity prediction: Lessons from D3R Grand Challenge 3. Journal of Computer-Aided Molecular Design, 2019, 33, 83-91.	1.3	23

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55	Cover Image, Volume 86, Issue S1. Proteins: Structure, Function and Bioinformatics, 2018, 86, C1.	1.5	2
56	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
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	A Membrane Protein Complex Docking Benchmark. Journal of Molecular Biology, 2018, 430, 5246-5256.	2.0	24
59	Distinguishing crystallographic from biological interfaces in protein complexes: role of intermolecular contacts and energetics for classification. BMC Bioinformatics, 2018, 19, 438.	1.2	25
60	Mapping the Contact Sites of the Escherichia coli Division-Initiating Proteins FtsZ and ZapA by BAMG Cross-Linking and Site-Directed Mutagenesis. International Journal of Molecular Sciences, 2018, 19, 2928.	1.8	11
61	INDIGO-DataCloud: a Platform to Facilitate Seamless Access to E-Infrastructures. Journal of Grid Computing, 2018, 16, 381-408.	2.5	58
62	HADDOCK. , 2018, , 1-3.		1
63	Defining distance restraints in HADDOCK. Nature Protocols, 2018, 13, 1503-1503.	5.5	18
64	Rapid Prediction of Multi-dimensional NMR Data Sets Using FANDAS. Methods in Molecular Biology, 2018, 1688, 111-132.	0.4	3
65	pdb-tools: a swiss army knife for molecular structures. F1000Research, 2018, 7, 1961.	0.8	99
66	Template-based proteinâ€“protein docking exploiting pairwise interfacial residue restraints. Briefings in Bioinformatics, 2017, 18, bbw027.	3.2	17
67	A benchmark testing ground for integrating homology modeling and protein docking. Proteins: Structure, Function and Bioinformatics, 2017, 85, 10-16.	1.5	29
68	The DisVis and PowerFit Web Servers: Explorative and Integrative Modeling of Biomolecular Complexes. Journal of Molecular Biology, 2017, 429, 399-407.	2.0	43
69	Information-Driven, Ensemble Flexible Peptide Docking Using HADDOCK. Methods in Molecular Biology, 2017, 1561, 109-138.	0.4	35
70	Prediction of Biomolecular Complexes. , 2017, , 265-292.		11
71	Prevention of VÎ³9VÎ´2 T Cell Activation by a VÎ³9VÎ´2 TCR Nanobody. Journal of Immunology, 2017, 198, 308-317.	0.4	9
72	Frontispiece: Supramolecular Organization and Functional Implications of K⁺â€...Channel Clusters in Membranes. Angewandte Chemie - International Edition, 2017, 56, .	7.2	0

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73	SpotOn: High Accuracy Identification of Protein-Protein Interface Hot-Spots. Scientific Reports, 2017, 7, 8007.	1.6	77
74	Supramolekulare Organisation und funktionale Auswirkungen von Ballungen von K⁺â€kanÃlen in Membranen. Angewandte Chemie, 2017, 129, 13404-13409.	1.6	1
75	Supramolecular Organization and Functional Implications of K⁺â€...Channel Clusters in Membranes. Angewandte Chemie - International Edition, 2017, 56, 13222-13227.	7.2	28
76	Membrane proteins structures: A review on computational modeling tools. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 2021-2039.	1.4	87
77	M3: an integrative framework for structure determination of molecular machines. Nature Methods, 2017, 14, 897-902.	9.0	39
78	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
79	Frontispiz: Supramolekulare Organisation und funktionale Auswirkungen von Ballungen von K⁺â€kanÃlen in Membranen. Angewandte Chemie, 2017, 129, .	1.6	0
80	PRODIGY: A Contact-based Predictor of Binding Affinity in Protein-protein Complexes. Bio-protocol, 2017, 7, e2124.	0.2	46
81	A Machine Learning Approach for Hot-Spot Detection at Protein-Protein Interfaces. International Journal of Molecular Sciences, 2016, 17, 1215.	1.8	46
82	dMM-PBSA: A New HADDOCK Scoring Function for Protein-Peptide Docking. Frontiers in Molecular Biosciences, 2016, 3, 46.	1.6	67
83	Novel Insights into Guide RNA 5â€²-Nucleoside/Tide Binding by Human Argonaute 2. International Journal of Molecular Sciences, 2016, 17, 22.	1.8	11
84	New Insight into the Catalytic Mechanism of Bacterial MraY from Enzyme Kinetics and Docking Studies. Journal of Biological Chemistry, 2016, 291, 15057-15068.	1.6	17
85	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
86	On the Combination of Restraint-Driven Docking of Flexible Peptides to Ion Channels - Lessons Learnt from the Complex Formed by the Spider Venom PcTx1 and the Acid Sensing Ion Channel1. Biophysical Journal, 2016, 110, 536a.	0.2	0
87	Defining the limits and reliability of rigid-body fitting in cryo-EM maps using multi-scale image pyramids. Journal of Structural Biology, 2016, 195, 252-258.	1.3	10
88	PRODIGY: a web server for predicting the binding affinity of proteinâ€“protein complexes. Bioinformatics, 2016, 32, 3676-3678.	1.8	760
89	Data publication with the structural biology data grid supports live analysis. Nature Communications, 2016, 7, 10882.	5.8	113
90	Structural basis of GM-CSF and IL-2 sequestration by the viral decoy receptor GIF. Nature Communications, 2016, 7, 13228.	5.8	15

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91	Structure of the bacterial plant-ferredoxin receptor FusA. Nature Communications, 2016, 7, 13308.	5.8	26
92	Exploring the interplay between experimental methods and the performance of predictors of binding affinity change upon mutations in protein complexes. Protein Engineering, Design and Selection, 2016, 29, 291-299.	1.0	26
93	Molecular dynamics characterization of the conformational landscape of small peptides: A series of handsâ€on collaborative practical sessions for undergraduate students. Biochemistry and Molecular Biology Education, 2016, 44, 160-167.	0.5	9
94	The solution structure of the kallikrein-related peptidases inhibitor SPINK6. Biochemical and Biophysical Research Communications, 2016, 471, 103-108.	1.0	7
95	Combination of Ambiguous and Unambiguous Data in the Restraint-driven Docking of Flexible Peptides with HADDOCK: The Binding of the Spider Toxin PcTx1 to the Acid Sensing Ion Channel (ASIC) 1a. Journal of Chemical Information and Modeling, 2016, 56, 127-138.	2.5	15
96	The HADDOCK2.2 Web Server: User-Friendly Integrative Modeling of Biomolecular Complexes. Journal of Molecular Biology, 2016, 428, 720-725.	2.0	2,071
97	Non-interacting surface solvation and dynamics in protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2015, 83, 445-458.	1.5	22
98	Structure-Function Relationships of Antimicrobial Peptides and Proteins with Respect to Contact Molecules on Pathogen Surfaces. Current Topics in Medicinal Chemistry, 2015, 16, 89-98.	1.0	18
99	Future opportunities and trends for e-infrastructures and life sciences: going beyond the grid to enable life science data analysis. Frontiers in Genetics, 2015, 6, 197.	1.1	8
100	Contacts-based prediction of binding affinity in proteinâ€“protein complexes. ELife, 2015, 4, e07454.	2.8	385
101	Dynamic binding mode of a Synaptotagmin-1â€“SNARE complex in solution. Nature Structural and Molecular Biology, 2015, 22, 555-564.	3.6	129
102	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
103	Probing a cell-embedded megadalton protein complex by DNP-supported solid-state NMR. Nature Methods, 2015, 12, 649-652.	9.0	124
104	DisVis: quantifying and visualizing accessible interaction space of distance-restrained biomolecular complexes. Bioinformatics, 2015, 31, 3222-3224.	1.8	61
105	Computational prediction of protein interfaces: A review of data driven methods. FEBS Letters, 2015, 589, 3516-3526.	1.3	148
106	Conformational Plasticity of the POTRA 5 Domain in the Outer Membrane Protein Assembly Factor BamA. Structure, 2015, 23, 1317-1324.	1.6	25
107	Information-Driven Structural Modelling of Proteinâ€“Protein Interactions. Methods in Molecular Biology, 2015, 1215, 399-424.	0.4	13
108	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. Structure, 2015, 23, 1156-1167.	1.6	159

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109	Integrative Modeling of Biomolecular Complexes: HADDOCKing with Cryo-Electron Microscopy Data. Structure, 2015, 23, 949-960.	1.6	69
110	Performance of the WeNMR CS-Rosetta3 web server in CASD-NMR. Journal of Biomolecular NMR, 2015, 62, 497-502.	1.6	9
111	Extended O-GlcNAc on HLA Class-I-Bound Peptides. Journal of the American Chemical Society, 2015, 137, 10922-10925.	6.6	72
112	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
113	Editorial overview: Proteinâ€“protein interactions. Current Opinion in Structural Biology, 2015, 35, vii-ix.	2.6	0
114	NMR-Based Modeling and Refinement of Protein 3D Structures. Methods in Molecular Biology, 2015, 1215, 351-380.	0.4	5
115	Information-Driven Modeling of Protein-Peptide Complexes. Methods in Molecular Biology, 2015, 1268, 221-239.	0.4	24
116	Fast and sensitive rigid-body fitting into cryo-EM density maps with PowerFit. AIMS Biophysics, 2015, 2, 73-87.	0.3	49
117	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
118	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
119	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
120	Integrative computational modeling of protein interactions. FEBS Journal, 2014, 281, 1988-2003.	2.2	94
121	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	1.5	50
122	Binding Hotspots of BAZ2B Bromodomain: Histone Interaction Revealed by Solution NMR Driven Docking. Biochemistry, 2014, 53, 6706-6716.	1.2	23
123	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
124	Mass Spec Studio for Integrative Structural Biology. Structure, 2014, 22, 1538-1548.	1.6	86
125	Information-driven modeling of large macromolecular assemblies using NMR data. Journal of Magnetic Resonance, 2014, 241, 103-114.	1.2	29
126	Sequence co-evolution gives 3D contacts and structures of protein complexes. ELife, 2014, 3, .	2.8	452

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127	Improving 3D structure prediction from chemical shift data. Journal of Biomolecular NMR, 2013, 57, 27-35.	1.6	25
128	Solvated proteinâ€“DNA docking using HADDOCK. Journal of Biomolecular NMR, 2013, 56, 51-63.	1.6	23
129	Defining the limits of homology modeling in informationâ€driven protein docking. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2119-2128.	1.5	63
130	Molecular origins of binding affinity: seeking the Archimedean point. Current Opinion in Structural Biology, 2013, 23, 868-877.	2.6	37
131	Advances in integrative modeling of biomolecular complexes. Methods, 2013, 59, 372-381.	1.9	67
132	Proteinâ€“protein interactions. Current Opinion in Structural Biology, 2013, 23, 859-861.	2.6	6
133	Solvated proteinâ€“protein docking using Kyteâ€Doolittleâ€based water preferences. Proteins: Structure, Function and Bioinformatics, 2013, 81, 510-518.	1.5	26
134	Structural Determinants of Specific Lipid Binding to Potassium Channels. Journal of the American Chemical Society, 2013, 135, 3983-3988.	6.6	73
135	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
136	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
137	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
138	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
139	Turning Defense into Offense: Defensin Mimetics as Novel Antibiotics Targeting Lipid II. PLoS Pathogens, 2013, 9, e1003732.	2.1	50
140	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
141	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
142	Unveiling the Interaction of Vanadium Compounds with Human Serum Albumin by Using1H STD NMR and Computational Docking Studies. European Journal of Inorganic Chemistry, 2013, 2013, 4619-4627.	1.0	18
143	A Unified Conformational Selection and Induced Fit Approach to Protein-Peptide Docking. PLoS ONE, 2013, 8, e58769.	1.1	163
144	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

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145	Dynamic Control of Selectivity in the Ubiquitination Pathway Revealed by an ASP to GLU Substitution in an Intra-Molecular Salt-Bridge Network. PLoS Computational Biology, 2012, 8, e1002754.	1.5	18
146	WeNMR: Structural Biology on the Grid. Journal of Grid Computing, 2012, 10, 743-767.	2.5	170
147	Rapid prediction of multi-dimensional NMR data sets. Journal of Biomolecular NMR, 2012, 54, 377-387.	1.6	35
148	SQUEEZE-E: The Optimal Solution for Molecular Simulations with Periodic Boundary Conditions. Journal of Chemical Theory and Computation, 2012, 8, 3618-3627.	2.3	6
149	MTMDAT-HADDOCK: High-throughput, protein complex structure modeling based on limited proteolysis and mass spectrometry. BMC Structural Biology, 2012, 12, 29.	2.3	11
150	Supramolecular Structure of Membrane-Associated Polypeptides by Combining Solid-State NMR and Molecular Dynamics Simulations. Biophysical Journal, 2012, 103, 29-37.	0.2	17
151	In support of the BMRB. Nature Structural and Molecular Biology, 2012, 19, 854-860.	3.6	6
152	Explicit Treatment of Water Molecules in Data-Driven Proteinâ€“Protein Docking: The Solvated HADDOCKing Approach. Methods in Molecular Biology, 2012, 819, 355-374.	0.4	20
153	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
154	Clustering biomolecular complexes by residue contacts similarity. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1810-1817.	1.5	103
155	A Flexible, Grid-Enabled Web Portal for GROMACS Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3463-3472.	2.3	32
156	Blind Testing of Routine, Fully Automated Determination of Protein Structures from NMR Data. Structure, 2012, 20, 227-236.	1.6	75
157	Predicting and dissecting high-order molecular complexity by information-driven biomolecular docking.. , 2012, , 232-246.		1
158	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
159	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	2.0	131
160	CPORT: A Consensus Interface Predictor and Its Performance in Prediction-Driven Docking with HADDOCK. PLoS ONE, 2011, 6, e17695.	1.1	272
161	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
162	Proteinâ€“protein HADDocking using exclusively pseudocontact shifts. Journal of Biomolecular NMR, 2011, 50, 263-266.	1.6	46

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163	NMR resonance assignments of NarE, a putative ADP-ribosylating toxin from Neisseria meningitidis. Biomolecular NMR Assignments, 2011, 5, 35-38.	0.4	5
164	1H, 13C and 15N assignment of the GNA1946 outer membrane lipoprotein from Neisseria meningitidis. Biomolecular NMR Assignments, 2011, 5, 135-138.	0.4	4
165	Quantitative use of chemical shifts for the modeling of protein complexes. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2662-2670.	1.5	20
166	A structureâ€based benchmark for proteinâ€“protein binding affinity. Protein Science, 2011, 20, 482-491.	3.1	252
167	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
168	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
169	Structural and Biochemical Characterization of NarE, an Iron-containing ADP-ribosyltransferase from Neisseria meningitidis. Journal of Biological Chemistry, 2011, 286, 14842-14851.	1.6	16
170	Adhesion/Growth-Regulatory Galectins: Insights into Their Ligand Selectivity Using Natural Glycoproteins and Glycotopes. Advances in Experimental Medicine and Biology, 2011, 705, 117-141.	0.8	8
171	The eNMR platform for structural biology. Journal of Structural and Functional Genomics, 2010, 11, 1-8.	1.2	18
172	SAMPLEX: Automatic mapping of perturbed and unperturbed regions of proteins and complexes. BMC Bioinformatics, 2010, 11, 51.	1.2	24
173	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
174	The HADDOCK web server for data-driven biomolecular docking. Nature Protocols, 2010, 5, 883-897.	5.5	1,167
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