Alexandre Bonvin

List of Publications by Year in Descending Order

277 papers	18,903 citations	65 h-index	130 g-index
328 ext. papers	22,480 ext. citations	6.8 avg, IF	6.99 L-index

#	Paper	IF	Citations
277	Molecular Insights Into Binding and Activation of the Human KCNQ2 Channel by Retigabine.. *Frontiers in Molecular Biosciences*, **2022**, 9, 839249	5.6	0
276	DeepRank: a deep learning framework for data mining 3D protein-protein interfaces. *Nature Communications*, **2021**, 12, 7068	17.4	3
275	Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. *Processes*, **2021**, 9, 71	2.9	34
274	Characterization of nucleosome sediments for protein interaction studies by solid-state NMR spectroscopy. *Magnetic Resonance*, **2021**, 2, 187-202	2.9	4
273	50 years of PBD: a catalyst in structural biology. *Nature Methods*, **2021**, 18, 448-449	21.6	2
272	Structural Biology in the Clouds: The WeNMR-EOSC Ecosystem. *Frontiers in Molecular Biosciences*, **2021**, 8, 729513	5.6	39
271	PDB-tools web: A user-friendly interface for the manipulation of PDB files. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 330-335	4.2	3
270	Integrating quantitative proteomics with accurate genome profiling of transcription factors by greenCUT&RUN. *Nucleic Acids Research*, **2021**, 49, e49	20.1	2
269	Shape-Restrained Modeling of Protein-Small-Molecule Complexes with High Ambiguity Driven DOCKing. *Journal of Chemical Information and Modeling*, **2021**, 61, 4807-4818	6.1	5
268	Native or Non-Native Protein-Protein Docking Models? Molecular Dynamics to the Rescue. *Journal of Chemical Theory and Computation*, **2021**, 17, 5944-5954	6.4	2
267	Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 1800-1823	4.2	17
266	Emergence and spread of SARS-CoV-2 lineage B.1.620 with variant of concern-like mutations and deletions. *Nature Communications*, **2021**, 12, 5769	17.4	14
265	Information-driven modeling of biomolecular complexes. *Current Opinion in Structural Biology*, **2021** , 70, 70-77	8.1	2
264	Coarse-grained (hybrid) integrative modeling of biomolecular interactions. *Computational and Structural Biotechnology Journal*, **2020**, 18, 1182-1190	6.8	9
263	Mode of action of teixobactins in cellular membranes. *Nature Communications*, **2020**, 11, 2848	17.4	28
262	Biological vs. Crystallographic Protein Interfaces: An Overview of Computational Approaches for Their Classification. *Crystals*, **2020**, 10, 114	2.3	6
261	A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo Community). *F1000Research*, **2020**, 9,	3.6	9

260	A click-flipped enzyme substrate boosts the performance of the diagnostic screening for Hunter syndrome. *Chemical Science*, **2020**, 11, 12671-12676	9.4	1
259	Understanding Docking Complexes of Macromolecules Using HADDOCK: The Synergy between Experimental Data and Computations. *Bio-protocol*, **2020**, 10, e3793	0.9	3
258	iScore: An MPI supported software for ranking protein-protein docking models based on a random walk graph kernel and support vector machines.. *SoftwareX*, **2020**, 11, 100462-100462	2.7	3
257	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	4.2	6
256	An overview of data-driven HADDOCK strategies in CAPRI rounds 38-45. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 1029-1036	4.2	6
255	Modeling Antibody-Antigen Complexes by Information-Driven Docking. *Structure*, **2020**, 28, 119-129.e2	5.2	19
254	Integrative Modelling of Biomolecular Complexes. *Journal of Molecular Biology*, **2020**, 432, 2861-2881	6.5	40
253	Inhibition of the integrated stress response by viral proteins that block p-eIF2-eIF2B association. *Nature Microbiology*, **2020**, 5, 1361-1373	26.6	17
252	Integrative modeling of membrane-associated protein assemblies. *Nature Communications*, **2020**, 11, 6210	17.4	9
251	Control over the fibrillization yield by varying the oligomeric nucleation propensities of self-assembling peptides. *Communications Chemistry*, **2020**, 3,	6.3	2
250	proABC-2: PRediction of AntiBody contacts v2 and its application to information-driven docking. *Bioinformatics*, **2020**, 36, 5107-5108	7.2	6
249	iScore: a novel graph kernel-based function for scoring protein-protein docking models. *Bioinformatics*, **2020**, 36, 112-121	7.2	27
248	Computational approaches to therapeutic antibody design: established methods and emerging trends. *Briefings in Bioinformatics*, **2020**, 21, 1549-1567	13.4	66
247	LightDock goes information-driven. *Bioinformatics*, **2020**, 36, 950-952	7.2	12
246	Pre- and post-docking sampling of conformational changes using ClustENM and HADDOCK for protein-protein and protein-DNA systems. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 292-306	4.2	21
245	The structural details of the interaction of single-stranded DNA binding protein hSSB2 (NABP1/OBFC2A) with UV-damaged DNA. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 319-326	4.2	6
244	Protein-Protein Modeling Using Cryo-EM Restraints. *Methods in Molecular Biology*, **2020**, 2112, 145-162	1.4	1
243	Sharing Data from Molecular Simulations. *Journal of Chemical Information and Modeling*, **2019**, 59, 4093-4099	4.9	11

242	Less Is More: Coarse-Grained Integrative Modeling of Large Biomolecular Assemblies with HADDOCK. *Journal of Chemical Theory and Computation*, **2019**, 15, 6358-6367	6.4	19
241	Folding Then Binding vs Folding Through Binding in Macrocyclic Peptide Inhibitors of Human Pancreatic □Amylase. *ACS Chemical Biology*, **2019**, 14, 1751-1759	4.9	10
240	PRODIGY-crystal: a web-tool for classification of biological interfaces in protein complexes. *Bioinformatics*, **2019**, 35, 4821-4823	7.2	9
239	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	6.1	22
238	Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 1200-1221	4.2	58
237	MARTINI-Based Protein-DNA Coarse-Grained HADDOCKing. *Frontiers in Molecular Biosciences*, **2019**, 6, 102	5.6	12
236	West-Life: A Virtual Research Environment for structural biology. *Journal of Structural Biology: X*, **2019**, 1, 100006	2.9	1
235	Large-scale prediction of binding affinity in protein-small ligand complexes: the PRODIGY-LIG web server. *Bioinformatics*, **2019**, 35, 1585-1587	7.2	48
234	Natural helix 9 mutants of PPAR□differently affect its transcriptional activity. *Molecular Metabolism*, **2019**, 20, 115-127	8.8	9
233	iSEE: Interface structure, evolution, and energy-based machine learning predictor of binding affinity changes upon mutations. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 110-119	4.2	33
232	Finding the □ spot: Are predictors of binding affinity changes upon mutations in protein□protein interactions ready for it?. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1410	7.9	32
231	Protein-ligand pose and affinity prediction: Lessons from D3R Grand Challenge 3. *Journal of Computer-Aided Molecular Design*, **2019**, 33, 83-91	4.2	15
230	Computational Tools for the Structural Characterization of Proteins and Their Complexes from Sequence-Evolutionary Data **2018**, 1-19		
229	Cover Image, Volume 86, Issue S1. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86, C1-C1	4.2	2
228	Assessment of contact predictions in CASP12: Co-evolution and deep learning coming of age. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86 Suppl 1, 51-66	4.2	126
227	Performance of HADDOCK and a simple contact-based protein-ligand binding affinity predictor in the D3R Grand Challenge 2. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 175-185	4.2	58
226	pdb-tools: a swiss army knife for molecular structures. *F1000Research*, **2018**, 7, 1961	3.6	25
225	Rapid Prediction of Multi-dimensional NMR Data Sets Using FANDAS. *Methods in Molecular Biology*, **2018**, 1688, 111-132	1.4	3

224	A Membrane Protein Complex Docking Benchmark. *Journal of Molecular Biology*, **2018**, 430, 5246-5256	6.5	17
223	Distinguishing crystallographic from biological interfaces in protein complexes: role of intermolecular contacts and energetics for classification. *BMC Bioinformatics*, **2018**, 19, 438	3.6	12
222	Mapping the Contact Sites of the Division-Initiating Proteins FtsZ and ZapA by BAMG Cross-Linking and Site-Directed Mutagenesis. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	7
221	INDIGO-DataCloud: a Platform to Facilitate Seamless Access to E-Infrastructures. *Journal of Grid Computing*, **2018**, 16, 381-408	4.2	44
220	Defining distance restraints in HADDOCK. *Nature Protocols*, **2018**, 13, 1503	18.8	11
219	A benchmark testing ground for integrating homology modeling and protein docking. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 10-16	4.2	24
218	The DisVis and PowerFit Web Servers: Explorative and Integrative Modeling of Biomolecular Complexes. *Journal of Molecular Biology*, **2017**, 429, 399-407	6.5	25
217	Information-Driven, Ensemble Flexible Peptide Docking Using HADDOCK. *Methods in Molecular Biology*, **2017**, 1561, 109-138	1.4	20
216	Prediction of Biomolecular Complexes **2017**, 265-292		5
215	Prevention of V9V2 T Cell Activation by a V9V2 TCR Nanobody. *Journal of Immunology*, **2017**, 198, 308-317	5.3	8
214	SpotOn: High Accuracy Identification of Protein-Protein Interface Hot-Spots. *Scientific Reports*, **2017**, 7, 8007	4.9	51
213	Supramolekulare Organisation und funktionale Auswirkungen von Ballungen von K+-Kanlen in Membranen. *Angewandte Chemie*, **2017**, 129, 13404-13409	3.6	1
212	Supramolecular Organization and Functional Implications of K Channel Clusters in Membranes. *Angewandte Chemie - International Edition*, **2017**, 56, 13222-13227	16.4	21
211	Membrane proteins structures: A review on computational modeling tools. *Biochimica Et Biophysica Acta - Biomembranes*, **2017**, 1859, 2021-2039	3.8	56
210	M3: an integrative framework for structure determination of molecular machines. *Nature Methods*, **2017**, 14, 897-902	21.6	30
209	Sense and simplicity in HADDOCK scoring: Lessons from CASP-CAPRI round 1. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 417-423	4.2	24
208	PRODIGY: A Contact-based Predictor of Binding Affinity in Protein-protein Complexes. *Bio-protocol*, **2017**, 7, e2124	0.9	16
207	Template-based protein-protein docking exploiting pairwise interfacial residue restraints. *Briefings in Bioinformatics*, **2017**, 18, 458-466	13.4	14

206	Data publication with the structural biology data grid supports live analysis. *Nature Communications*, **2016**, 7, 10882	17.4	78
205	Structural basis of GM-CSF and IL-2 sequestration by the viral decoy receptor GIF. *Nature Communications*, **2016**, 7, 13228	17.4	11
204	Structure of the bacterial plant-ferredoxin receptor FusA. *Nature Communications*, **2016**, 7, 13308	17.4	22
203	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	1.9	16
202	Molecular dynamics characterization of the conformational landscape of small peptides: A series of hands-on collaborative practical sessions for undergraduate students. *Biochemistry and Molecular Biology Education*, **2016**, 44, 160-7	1.3	8
201	The solution structure of the kallikrein-related peptidases inhibitor SPINK6. *Biochemical and Biophysical Research Communications*, **2016**, 471, 103-8	3.4	6
200	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, 127-38	6.1	6
199	The HADDOCK2.2 Web Server: User-Friendly Integrative Modeling of Biomolecular Complexes. *Journal of Molecular Biology*, **2016**, 428, 720-725	6.5	1155
198	Structure-Function Relationships of Antimicrobial Peptides and Proteins with Respect to Contact Molecules on Pathogen Surfaces. *Current Topics in Medicinal Chemistry*, **2016**, 16, 89-98	3	16
197	A Machine Learning Approach for Hot-Spot Detection at Protein-Protein Interfaces. *International Journal of Molecular Sciences*, **2016**, 17,	6.3	33
196	dMM-PBSA: A New HADDOCK Scoring Function for Protein-Peptide Docking. *Frontiers in Molecular Biosciences*, **2016**, 3, 46	5.6	42
195	New Insight into the Catalytic Mechanism of Bacterial MraY from Enzyme Kinetics and Docking Studies. *Journal of Biological Chemistry*, **2016**, 291, 15057-68	5.4	15
194	Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84 Suppl 1, 323-48	4.2	111
193	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	3.4	9
192	PRODIGY: a web server for predicting the binding affinity of protein-protein complexes. *Bioinformatics*, **2016**, 32, 3676-3678	7.2	272
191	Conformational Plasticity of the POTRA 5 Domain in the Outer Membrane Protein Assembly Factor BamA. *Structure*, **2015**, 23, 1317-24	5.2	19
190	Information-driven structural modelling of protein-protein interactions. *Methods in Molecular Biology*, **2015**, 1215, 399-424	1.4	7
189	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. *Structure*, **2015**, 23, 1156-67	5.2	131

188	Integrative Modeling of Biomolecular Complexes: HADDOCKing with Cryo-Electron Microscopy Data. *Structure*, **2015**, 23, 949-960	5.2	49
187	Performance of the WeNMR CS-Rosetta3 web server in CASD-NMR. *Journal of Biomolecular NMR*, **2015**, 62, 497-502	3	8
186	Extended O-GlcNAc on HLA Class-I-Bound Peptides. *Journal of the American Chemical Society*, **2015**, 137, 10922-10925	16.4	60
185	Updates to the Integrated Protein-Protein Interaction Benchmarks: Docking Benchmark Version 5 and Affinity Benchmark Version 2. *Journal of Molecular Biology*, **2015**, 427, 3031-41	6.5	208
184	Non-interacting surface solvation and dynamics in protein-protein interactions. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 445-58	4.2	20
183	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	4.5	7
182	Contacts-based prediction of binding affinity in protein-protein complexes. *ELife*, **2015**, 4, e07454	8.9	190
181	Dynamic binding mode of a Synaptotagmin-1-SNARE complex in solution. *Nature Structural and Molecular Biology*, **2015**, 22, 555-64	17.6	99
180	The Supramolecular Organization of a Peptide-Based Nanocarrier at High Molecular Detail. *Journal of the American Chemical Society*, **2015**, 137, 7775-84	16.4	42
179	Probing a cell-embedded megadalton protein complex by DNP-supported solid-state NMR. *Nature Methods*, **2015**, 12, 649-52	21.6	103
178	DisVis: quantifying and visualizing accessible interaction space of distance-restrained biomolecular complexes. *Bioinformatics*, **2015**, 31, 3222-4	7.2	37
177	Computational prediction of protein interfaces: A review of data driven methods. *FEBS Letters*, **2015**, 589, 3516-26	3.8	96
176	Fast and sensitive rigid-body fitting into cryo-EM density maps with PowerFit. *AIMS Biophysics*, **2015** , 2, 73-87	0.8	26
175	Author response: Contacts-based prediction of binding affinity in protein–protein complexes **2015**,		2
174	NMR-based modeling and refinement of protein 3D structures. *Methods in Molecular Biology*, **2015**, 1215, 351-80	1.4	4
173	Information-driven modeling of protein-peptide complexes. *Methods in Molecular Biology*, **2015**, 1268, 221-39	1.4	16
172	Novel Insights into Guide RNA 5′-Nucleoside/Tide Binding by Human Argonaute 2. *International Journal of Molecular Sciences*, **2015**, 17,	6.3	5
171	Integrative computational modeling of protein interactions. *FEBS Journal*, **2014**, 281, 1988-2003	5.7	77

170	Blind prediction of interfacial water positions in CAPRI. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 620-32	4.2	43
169	Binding hotspots of BAZ2B bromodomain: Histone interaction revealed by solution NMR driven docking. *Biochemistry*, **2014**, 53, 6706-16	3.2	18
168	HADDOCK(2P2I): a biophysical model for predicting the binding affinity of protein-protein interaction inhibitors. *Journal of Chemical Information and Modeling*, **2014**, 54, 826-36	6.1	24
167	Mass spec studio for integrative structural biology. *Structure*, **2014**, 22, 1538-48	5.2	66
166	Information-driven modeling of large macromolecular assemblies using NMR data. *Journal of Magnetic Resonance*, **2014**, 241, 103-14	3	24
165	Insight into cyanobacterial circadian timing from structural details of the KaiB-KaiC interaction. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 1379-84	11.5	49
164	Modeling protein-protein complexes using the HADDOCK webserver "modeling protein complexes with HADDOCK". *Methods in Molecular Biology*, **2014**, 1137, 163-79	1.4	31
163	Proteins feel more than they see: fine-tuning of binding affinity by properties of the non-interacting surface. *Journal of Molecular Biology*, **2014**, 426, 2632-52	6.5	69
162	Sequence co-evolution gives 3D contacts and structures of protein complexes. *ELife*, **2014**, 3,	8.9	324
161	Author response: Sequence co-evolution gives 3D contacts and structures of protein complexes **2014**,		2
160	Improving 3D structure prediction from chemical shift data. *Journal of Biomolecular NMR*, **2013**, 57, 27-35	3	23
159	Solvated protein-DNA docking using HADDOCK. *Journal of Biomolecular NMR*, **2013**, 56, 51-63	3	18
158	Defining the limits of homology modeling in information-driven protein docking. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 2119-28	4.2	47
157	Molecular origins of binding affinity: seeking the Archimedean point. *Current Opinion in Structural Biology*, **2013**, 23, 868-77	8.1	34
156	Advances in integrative modeling of biomolecular complexes. *Methods*, **2013**, 59, 372-81	4.6	57
155	Solvated protein-protein docking using Kyte-Doolittle-based water preferences. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 510-8	4.2	23
154	Structural determinants of specific lipid binding to potassium channels. *Journal of the American Chemical Society*, **2013**, 135, 3983-8	16.4	65
153	Importance of lipid-pore loop interface for potassium channel structure and function. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 13008-13	11.5	42

152	Short-chain fatty acids stimulate angiopoietin-like 4 synthesis in human colon adenocarcinoma cells by activating peroxisome proliferator-activated receptor □*Molecular and Cellular Biology*, **2013**, 33, 1303-16	4.8	156
151	On the binding affinity of macromolecular interactions: daring to ask why proteins interact. *Journal of the Royal Society Interface*, **2013**, 10, 20120835	4.1	251
150	A gp41 MPER-specific llama VHH requires a hydrophobic CDR3 for neutralization but not for antigen recognition. *PLoS Pathogens*, **2013**, 9, e1003202	7.6	52
149	Turning defense into offense: defensin mimetics as novel antibiotics targeting lipid II. *PLoS Pathogens*, **2013**, 9, e1003732	7.6	41
148	Gentamicin binds to the megalin receptor as a competitive inhibitor using the common ligand binding motif of complement type repeats: insight from the nmr structure of the 10th complement type repeat domain alone and in complex with gentamicin. *Journal of Biological Chemistry*, **2013**, 288, 4424-35	5.4	39
147	On the usefulness of ion-mobility mass spectrometry and SAXS data in scoring docking decoys. *Acta Crystallographica Section D: Biological Crystallography*, **2013**, 69, 683-94		50
146	Unveiling the Interaction of Vanadium Compounds with Human Serum Albumin by Using 1H STD NMR and Computational Docking Studies. *European Journal of Inorganic Chemistry*, **2013**, 2013, 4619-4627	2.3	16
145	A unified conformational selection and induced fit approach to protein-peptide docking. *PLoS ONE*, **2013**, 8, e58769	3.7	132
144	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 1980-7	4.2	78
143	Blind testing of routine, fully automated determination of protein structures from NMR data. *Structure*, **2012**, 20, 227-36	5.2	64
142	WeNMR: Structural Biology on the Grid. *Journal of Grid Computing*, **2012**, 10, 743-767	4.2	142
141	Rapid prediction of multi-dimensional NMR data sets. *Journal of Biomolecular NMR*, **2012**, 54, 377-87	3	32
140	SQUEEZE-E: The Optimal Solution for Molecular Simulations with Periodic Boundary Conditions. *Journal of Chemical Theory and Computation*, **2012**, 8, 3618-27	6.4	5
139	MTMDAT-HADDOCK: high-throughput, protein complex structure modeling based on limited proteolysis and mass spectrometry. *BMC Structural Biology*, **2012**, 12, 29	2.7	11
138	Supramolecular structure of membrane-associated polypeptides by combining solid-state NMR and molecular dynamics simulations. *Biophysical Journal*, **2012**, 103, 29-37	2.9	16
137	In support of the BMRB. *Nature Structural and Molecular Biology*, **2012**, 19, 854-60	17.6	5
136	Explicit treatment of water molecules in data-driven protein-protein docking: the solvated HADDOCKing approach. *Methods in Molecular Biology*, **2012**, 819, 355-74	1.4	20
135	Next challenges in protein□protein docking: from proteome to interactome and beyond. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 642-651	7.9	22

134	Clustering biomolecular complexes by residue contacts similarity. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 1810-7	4.2	69
133	A Flexible, Grid-Enabled Web Portal for GROMACS Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2012**, 8, 3463-72	6.4	25
132	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	5	15
131	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, 150-61	4	66
130	Community-wide assessment of protein-interface modeling suggests improvements to design methodology. *Journal of Molecular Biology*, **2011**, 414, 289-302	6.5	114
129	CPORT: a consensus interface predictor and its performance in prediction-driven docking with HADDOCK. *PLoS ONE*, **2011**, 6, e17695	3.7	188
128	A multidomain flexible docking approach to deal with large conformational changes in the modeling of biomolecular complexes. *Structure*, **2011**, 19, 555-65	5.2	52
127	Protein-protein HADDocking using exclusively pseudocontact shifts. *Journal of Biomolecular NMR*, **2011**, 50, 263-6	3	42
126	NMR resonance assignments of NarE, a putative ADP-ribosylating toxin from Neisseria meningitidis. *Biomolecular NMR Assignments*, **2011**, 5, 35-8	0.7	5
125	1H, 13C and 15N assignment of the GNA1946 outer membrane lipoprotein from Neisseria meningitidis. *Biomolecular NMR Assignments*, **2011**, 5, 135-8	0.7	1
124	Quantitative use of chemical shifts for the modeling of protein complexes. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2662-70	4.2	18
123	A structure-based benchmark for protein-protein binding affinity. *Protein Science*, **2011**, 20, 482-91	6.3	194
122	Characterizing the N- and C-terminal Small ubiquitin-like modifier (SUMO)-interacting motifs of the scaffold protein DAXX. *Journal of Biological Chemistry*, **2011**, 286, 19816-29	5.4	27
121	Antimicrobial and efflux pump inhibitory activity of caffeoylquinic acids from Artemisia absinthium against gram-positive pathogenic bacteria. *PLoS ONE*, **2011**, 6, e18127	3.7	104
120	Structural and biochemical characterization of NarE, an iron-containing ADP-ribosyltransferase from Neisseria meningitidis. *Journal of Biological Chemistry*, **2011**, 286, 14842-51	5.4	16
119	Adhesion/growth-regulatory galectins: insights into their ligand selectivity using natural glycoproteins and glycotopes. *Advances in Experimental Medicine and Biology*, **2011**, 705, 117-41	3.6	7
118	The HADDOCK web server for data-driven biomolecular docking. *Nature Protocols*, **2010**, 5, 883-97	18.8	936
117	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	5.4	25

116	Building macromolecular assemblies by information-driven docking: introducing the HADDOCK multibody docking server. *Molecular and Cellular Proteomics*, **2010**, 9, 1784-94	7.6	98
115	Pushing the limits of what is achievable in protein-DNA docking: benchmarking HADDOCK© performance. *Nucleic Acids Research*, **2010**, 38, 5634-47	20.1	41
114	Plectasin, a fungal defensin, targets the bacterial cell wall precursor Lipid II. *Science*, **2010**, 328, 1168-72	33.3	400
113	Are scoring functions in protein-protein docking ready to predict interactomes? Clues from a novel binding affinity benchmark. *Journal of Proteome Research*, **2010**, 9, 2216-25	5.6	196
112	Data-driven Docking: Using External Information to Spark the Biomolecular Rendez-vous **2010**, 182-208		6
111	The eNMR platform for structural biology. *Journal of Structural and Functional Genomics*, **2010**, 11, 1-8		17
110	SAMPLEX: automatic mapping of perturbed and unperturbed regions of proteins and complexes. *BMC Bioinformatics*, **2010**, 11, 51	3.6	22
109	Strengths and weaknesses of data-driven docking in critical assessment of prediction of interactions. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 3242-9	4.2	35
108	Understanding the role of the Josephin domain in the PolyUb binding and cleavage properties of ataxin-3. *PLoS ONE*, **2010**, 5, e12430	3.7	49
107	Detailed mechanistic insights into HIV-1 sensitivity to three generations of fusion inhibitors. *Journal of Biological Chemistry*, **2009**, 284, 26941-50	5.4	64
106	3D-DART: a DNA structure modelling server. *Nucleic Acids Research*, **2009**, 37, W235-9	20.1	262
105	A comprehensive framework of E2-RING E3 interactions of the human ubiquitin-proteasome system. *Molecular Systems Biology*, **2009**, 5, 295	12.2	108
104	A comprehensive framework of E2RING E3 interactions of the human ubiquitinproteasome system. *Molecular Systems Biology*, **2009**, 5, 317	12.2	19
103	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, 1960-4	11.5	34
102	MINOES: a new approach to select a representative ensemble of structures in NMR studies of (partially) unfolded states. Application to Delta25-PYP. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 895-904	4.2	13
101	Insights into the DNA cleavage mechanism of human LINE-1 retrotransposon endonuclease. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 917-28	4.2	3
100	CASD-NMR: critical assessment of automated structure determination by NMR. *Nature Methods*, **2009**, 6, 625-6	21.6	51
99	Data-driven homology modelling of P-glycoprotein in the ATP-bound state indicates flexibility of the transmembrane domains. *FEBS Journal*, **2009**, 276, 964-72	5.7	32

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List of Publications

8	Information-Driven Modelling of Antibody-Antigen Complexes. *SSRN Electronic Journal*,	1	1
7	proABC-2: PRediction Of AntiBody Contacts v2 and its application to information-driven docking		2
6	An enhanced-sampling MD-based protocol for molecular docking		1
5	iScore: A novel graph kernel-based function for scoring protein-protein docking models		1
4	Less is more: Coarse-grained integrative modeling of large biomolecular assemblies with HADDOCK		1
3	Cryptic pathogen-sugar interactions revealed by universal saturation transfer analysis		5
2	Travel-driven emergence and spread of SARS-CoV-2 lineage B.1.620 with multiple VOC-like mutations and deletions in Europe		11
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