Alexandre Bonvin

List of Publications by Citations

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	HADDOCK: a protein-protein docking approach based on biochemical or biophysical information. *Journal of the American Chemical Society*, **2003**, 125, 1731-7	16.4	2126
276	The HADDOCK2.2 Web Server: User-Friendly Integrative Modeling of Biomolecular Complexes. *Journal of Molecular Biology*, **2016**, 428, 720-725	6.5	1155
275	The HADDOCK web server for data-driven biomolecular docking. *Nature Protocols*, **2010**, 5, 883-97	18.8	936
274	Refinement of protein structures in explicit solvent. *Proteins: Structure, Function and Bioinformatics*, **2003**, 50, 496-506	4.2	521
273	HADDOCK versus HADDOCK: new features and performance of HADDOCK2.0 on the CAPRI targets. *Proteins: Structure, Function and Bioinformatics*, **2007**, 69, 726-33	4.2	462
272	Structure and flexibility adaptation in nonspecific and specific protein-DNA complexes. *Science*, **2004**, 305, 386-9	33.3	454
271	The nisin-lipid II complex reveals a pyrophosphate cage that provides a blueprint for novel antibiotics. *Nature Structural and Molecular Biology*, **2004**, 11, 963-7	17.6	438
270	Plectasin, a fungal defensin, targets the bacterial cell wall precursor Lipid II. *Science*, **2010**, 328, 1168-72	33.3	400
269	Structural basis for signal-sequence recognition by the translocase motor SecA as determined by NMR. *Cell*, **2007**, 131, 756-69	56.2	337
268	Sequence co-evolution gives 3D contacts and structures of protein complexes. *ELife*, **2014**, 3,	8.9	324
267	The alpha-to-beta conformational transition of Alzheimer© Abeta-(1-42) peptide in aqueous media is reversible: a step by step conformational analysis suggests the location of beta conformation seeding. *ChemBioChem*, **2006**, 7, 257-67	3.8	314
266	RECOORD: a recalculated coordinate database of 500+ proteins from the PDB using restraints from the BioMagResBank. *Proteins: Structure, Function and Bioinformatics*, **2005**, 59, 662-72	4.2	285
265	PRODIGY: a web server for predicting the binding affinity of protein-protein complexes. *Bioinformatics*, **2016**, 32, 3676-3678	7.2	272
264	3D-DART: a DNA structure modelling server. *Nucleic Acids Research*, **2009**, 37, W235-9	20.1	262
263	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
262	Flexible protein-protein docking. *Current Opinion in Structural Biology*, **2006**, 16, 194-200	8.1	242
261	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

260	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
259	A structure-based benchmark for protein-protein binding affinity. *Protein Science*, **2011**, 20, 482-91	6.3	194
258	Contacts-based prediction of binding affinity in protein-protein complexes. *ELife*, **2015**, 4, e07454	8.9	190
257	CPORT: a consensus interface predictor and its performance in prediction-driven docking with HADDOCK. *PLoS ONE*, **2011**, 6, e17695	3.7	188
256	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
255	Information-driven protein-DNA docking using HADDOCK: it is a matter of flexibility. *Nucleic Acids Research*, **2006**, 34, 3317-25	20.1	148
254	WeNMR: Structural Biology on the Grid. *Journal of Grid Computing*, **2012**, 10, 743-767	4.2	142
253	A unified conformational selection and induced fit approach to protein-peptide docking. *PLoS ONE*, **2013**, 8, e58769	3.7	132
252	Outcome of the First wwPDB Hybrid/Integrative Methods Task Force Workshop. *Structure*, **2015**, 23, 1156-67	5.2	131
251	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
250	Solvated docking: introducing water into the modelling of biomolecular complexes. *Bioinformatics*, **2006**, 22, 2340-7	7.2	123
249	Conformational variability of solution nuclear magnetic resonance structures. *Journal of Molecular Biology*, **1995**, 250, 80-93	6.5	117
248	WHISCY: what information does surface conservation yield? Application to data-driven docking. *Proteins: Structure, Function and Bioinformatics*, **2006**, 63, 479-89	4.2	115
247	Community-wide assessment of protein-interface modeling suggests improvements to design methodology. *Journal of Molecular Biology*, **2011**, 414, 289-302	6.5	114
246	Data-driven docking for the study of biomolecular complexes. *FEBS Journal*, **2005**, 272, 293-312	5.7	112
245	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
244	A comprehensive framework of E2-RING E3 interactions of the human ubiquitin-proteasome system. *Molecular Systems Biology*, **2009**, 5, 295	12.2	108
243	NMR study of mersacidin and lipid II interaction in dodecylphosphocholine micelles. Conformational changes are a key to antimicrobial activity. *Journal of Biological Chemistry*, **2003**, 278, 13110-7	5.4	105

242	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
241	Probing a cell-embedded megadalton protein complex by DNP-supported solid-state NMR. *Nature Methods*, **2015**, 12, 649-52	21.6	103
240	Structural model of the UbcH5B/CNOT4 complex revealed by combining NMR, mutagenesis, and docking approaches. *Structure*, **2004**, 12, 633-44	5.2	103
239	Plasticity in protein-DNA recognition: lac repressor interacts with its natural operator 01 through alternative conformations of its DNA-binding domain. *EMBO Journal*, **2002**, 21, 2866-76	13	103
238	Dynamic binding mode of a Synaptotagmin-1-SNARE complex in solution. *Nature Structural and Molecular Biology*, **2015**, 22, 555-64	17.6	99
237	The solution structure of the AppA BLUF domain: insight into the mechanism of light-induced signaling. *ChemBioChem*, **2006**, 7, 187-93	3.8	99
236	NMR analysis of protein interactions. *Current Opinion in Chemical Biology*, **2005**, 9, 501-8	9.7	99
235	Building macromolecular assemblies by information-driven docking: introducing the HADDOCK multibody docking server. *Molecular and Cellular Proteomics*, **2010**, 9, 1784-94	7.6	98
234	Computational prediction of protein interfaces: A review of data driven methods. *FEBS Letters*, **2015**, 589, 3516-26	3.8	96
233	How proteins get in touch: interface prediction in the study of biomolecular complexes. *Current Protein and Peptide Science*, **2008**, 9, 394-406	2.8	94
232	Hydramacin-1, structure and antibacterial activity of a protein from the basal metazoan Hydra. *Journal of Biological Chemistry*, **2009**, 284, 1896-905	5.4	90
231	Hydration dynamics of the collagen triple helix by NMR. *Journal of Molecular Biology*, **2000**, 300, 1041-9	6.5	86
230	DRESS: a database of REfined solution NMR structures. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 483-6	4.2	83
229	beta-hairpin stability and folding: molecular dynamics studies of the first beta-hairpin of tendamistat. *Journal of Molecular Biology*, **2000**, 296, 255-68	6.5	82
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226	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
225	Integrative computational modeling of protein interactions. *FEBS Journal*, **2014**, 281, 1988-2003	5.7	77

224	Water molecules in DNA recognition II: a molecular dynamics view of the structure and hydration of the trp operator. *Journal of Molecular Biology*, **1998**, 282, 859-73	6.5	75
223	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, 367-81	4.2	72
222	The solution structure of Lac repressor headpiece 62 complexed to a symmetrical lac operator. *Structure*, **1999**, 7, 1483-92	5.2	72
221	Data-driven docking: HADDOCK© adventures in CAPRI. *Proteins: Structure, Function and Bioinformatics*, **2005**, 60, 232-8	4.2	70
220	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
219	Clustering biomolecular complexes by residue contacts similarity. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 1810-7	4.2	69
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208	Nuclear magnetic resonance solution structure of the Arc repressor using relaxation matrix calculations. *Journal of Molecular Biology*, **1994**, 236, 328-41	6.5	64
207	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, 7071-6	11.5	63

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205	Extended O-GlcNAc on HLA Class-I-Bound Peptides. *Journal of the American Chemical Society*, **2015**, 137, 10922-10925	16.4	60
204	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
203	Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 1200-1221	4.2	58
202	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. *Glycobiology*, **2007**, 17, 165-84	5.8	58
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193	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
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183	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
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181	The solution structure of the human retinoic acid receptor-beta DNA-binding domain. *Journal of Biomolecular NMR*, **1993**, 3, 1-17	3	49
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169	dMM-PBSA: A New HADDOCK Scoring Function for Protein-Peptide Docking. *Frontiers in Molecular Biosciences*, **2016**, 3, 46	5.6	42
168	Turning defense into offense: defensin mimetics as novel antibiotics targeting lipid II. *PLoS Pathogens*, **2013**, 9, e1003732	7.6	41
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157	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
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110	A comprehensive framework of E2-RING E3 interactions of the human ubiquitin-proteasome system. *Molecular Systems Biology*, **2009**, 5, 317	12.2	19
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