Juan Fernandez-Recio

List of Publications by Year
in descending order

132	6,945	47006	71685
papers	citations	47 h-index	76 g-index

140	140	140	6929
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	4.2	348
2	pyDock: Electrostatics and desolvation for effective scoring of rigid-body protein-protein docking. Proteins: Structure, Function and Bioinformatics, 2007, 68, 503-515.	2.6	286
3	Identification of Proteinâ€“Protein Interaction Sites from Docking Energy Landscapes. Journal of Molecular Biology, 2004, 335, 843-865.	4.2	276
4	SwarmDock: a server for flexible proteinâ€“protein docking. Bioinformatics, 2013, 29, 807-809.	4.1	259
5	SKEMPI: a Structural Kinetic and Energetic database of Mutant Protein Interactions and its use in empirical models. Bioinformatics, 2012, 28, 2600-2607.	4.1	237
6	pyDockWEB: a web server for rigid-body proteinâ€“protein docking using electrostatics and desolvation scoring. Bioinformatics, 2013, 29, 1698-1699.	4.1	214
7	SKEMPI 2.0: an updated benchmark of changes in proteinâ€“protein binding energy, kinetics and thermodynamics upon mutation. Bioinformatics, 2019, 35, 462-469.	4.1	191
8	Optimal docking area: A new method for predicting protein-protein interaction sites. Proteins: Structure, Function and Bioinformatics, 2004, 58, 134-143.	2.6	185
9	ICM-DISCO docking by global energy optimization with fully flexible side-chains. Proteins: Structure, Function and Bioinformatics, 2003, 52, 113-117.	2.6	183
10	Soft protein-protein docking in internal coordinates. Protein Science, 2009, 11, 280-291.	7.6	175
11	Assembly and Channel Opening in a Bacterial Drug Efflux Machine. Molecular Cell, 2008, 30, 114-121.	9.7	155
12	Polygalacturonase inhibiting proteins: players in plant innate immunity?. Trends in Plant Science, 2006, 11, 65-70.	8.8	153
13	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.	2.6	148
14	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	4.2	131
15	FRODOCK: a new approach for fast rotational proteinâ€“protein docking. Bioinformatics, 2009, 25, 2544-2551.	4.1	126
16	The Crystal Structure of Fibroblast Growth Factor (FGF) 19 Reveals Novel Features of the FGF Family and Offers a Structural Basis for Its Unusual Receptor Affinityâ€‚â€¡. Biochemistry, 2004, 43, 629-640.	2.5	116
17	Identification of hot-spot residues in protein-protein interactions by computational docking. BMC Bioinformatics, 2008, 9, 447.	2.6	107
18	The Tryptophan/Histidine interaction in Î±-helices. Journal of Molecular Biology, 1997, 267, 184-197.	4.2	101

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19	The Structure of Human 4F2hc Ectodomain Provides a Model for Homodimerization and Electrostatic Interaction with Plasma Membrane. Journal of Biological Chemistry, 2007, 282, 31444-31452.	3.4	101
20	Blind prediction of homoâ€•and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	2.6	99
21	The scoring of poses in protein-protein docking: current capabilities and future directions. BMC Bioinformatics, 2013, 14, 286.	2.6	98
22	The Crystal Structure of the Outer Membrane Protein VceC from the Bacterial Pathogen Vibrio cholerae at 1.8 Ã... Resolution. Journal of Biological Chemistry, 2005, 280, 15307-15314.	3.4	91
23	Scoring functions for proteinâ€“protein interactions. Current Opinion in Structural Biology, 2013, 23, 862-867.	5.7	87
24	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1980-1987.	2.6	87
25	Structural bases for the interaction and stabilization of the human amino acid transporter LAT2 with its ancillary protein 4F2hc. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 2966-2971.	7.1	84
26	Optimal proteinâ€RNA area, OPRA: A propensityâ€based method to identify RNAâ€binding sites on proteins. Proteins: Structure, Function and Bioinformatics, 2010, 78, 25-35.	2.6	83
27	LightDock: a new multi-scale approach to proteinâ€“protein docking. Bioinformatics, 2018, 34, 49-55.	4.1	83
28	Present and future challenges and limitations in proteinâ€“protein docking. Proteins: Structure, Function and Bioinformatics, 2010, 78, 95-108.	2.6	76
29	Energetics of a hydrogen bond (charged and neutral) and of a cation-Ï€ interaction in apoflavodoxin 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 1999, 290, 319-330.	4.2	73
30	Prediction of protein assemblies, the next frontier: The <scp>CASP14â€CAPRI</scp> experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1800-1823.	2.6	73
31	The Crystal Structure of the BAR Domain from Human Bin1/Amphiphysin II and Its Implications for Molecular Recognitionâ€. Biochemistry, 2006, 45, 12917-12928.	2.5	72
32	A model of a transmembrane drug-efflux pump from Gram-negative bacteria. FEBS Letters, 2004, 578, 5-9.	2.8	71
33	Scoring by Intermolecular Pairwise Propensities of Exposed Residues (SIPPER): A New Efficient Potential for Proteinâ^'Protein Docking. Journal of Chemical Information and Modeling, 2011, 51, 370-377.	5.4	70
34	Integration of evolutionary and desolvation energy analysis identifies functional sites in a plant immunity protein. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 7666-7671.	7.1	68
35	Pushing Structural Information into the Yeast Interactome by High-Throughput Protein Docking Experiments. PLoS Computational Biology, 2009, 5, e1000490.	3.2	67
36	Recognition and Cooperation Between the ATP-dependent RNA Helicase RhlB and Ribonuclease RNase E. Journal of Molecular Biology, 2007, 367, 113-132.	4.2	66

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37	Structural Characterization of Proteinâ€“Protein Complexes by Integrating Computational Docking with Small-angle Scattering Data. Journal of Molecular Biology, 2010, 403, 217-230.	4.2	64
38	Hot-spot analysis for drug discovery targeting protein-protein interactions. Expert Opinion on Drug Discovery, 2018, 13, 327-338.	5.0	64
39	Modulation of Electroenzymatic NADPH Oxidation through Oriented Immobilization of Ferredoxin:NADP+Reductase onto Modified Gold Electrodes. Journal of the American Chemical Society, 2000, 122, 9808-9817.	13.7	63
40	pyDockSAXS: proteinâ€“protein complex structure by SAXS and computational docking. Nucleic Acids Research, 2015, 43, W356-W361.	14.5	61
41	CCharPPI web server: computational characterization of proteinâ€“protein interactions from structure. Bioinformatics, 2015, 31, 123-125.	4.1	61
42	Efficient Restraints for Proteinâ€“Protein Docking by Comparison of Observed Amino Acid Substitution Patterns with those Predicted from Local Environment. Journal of Molecular Biology, 2006, 357, 1669-1682.	4.2	58
43	Allosteric Conversation in the Androgen Receptor Ligand-Binding Domain Surfaces. Molecular Endocrinology, 2012, 26, 1078-1090.	3.7	58
44	Established and Emerging Trends in Computational Drug Discovery in the Structural Genomics Era. Chemistry and Biology, 2012, 19, 29-41.	6.0	57
45	L amino acid transporter structure and molecular bases for the asymmetry of substrate interaction. Nature Communications, 2019, 10, 1807.	12.8	57
46	The Polygalacturonase-Inhibiting Protein PGIP2 of Phaseolus vulgaris Has Evolved a Mixed Mode of Inhibition of Endopolygalacturonase PG1 of Botrytis cinerea. Plant Physiology, 2005, 139, 1380-1388.	4.8	53
47	Identifying interaction motifs in CK2Î² â€“ a ubiquitous kinase regulatory subunit. Trends in Biochemical Sciences, 2006, 31, 654-661.	7.5	51
48	Prediction of protein binding sites and hot spots. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 680-698.	14.6	50
49	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	2.6	50
50	Brief encounters bolster contacts. Nature, 2006, 444, 279-280.	27.8	46
51	LRR Conservation Mapping to Predict Functional Sites within Protein Leucine-Rich Repeat Domains. PLoS ONE, 2011, 6, e21614.	2.5	46
52	Prediction of protein-binding areas by small-world residue networks and application to docking. BMC Bioinformatics, 2011, 12, 378.	2.6	46
53	A proteinâ€RNA docking benchmark (II): Extended set from experimental and homology modeling data. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1872-1882.	2.6	46
54	Structural basis for the recruitment and activation of the Legionella phospholipase VipD by the host GTPase Rab5. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E3514-23.	7.1	46

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55	Improving CAPRI predictions: Optimized desolvation for rigid-body docking. Proteins: Structure, Function and Bioinformatics, 2005, 60, 308-313.	2.6	45
56	Crystal structure of the endopolygalacturonase from the phytopathogenic fungus Colletotrichum lupini and its interaction with polygalacturonaseâ€inhibiting proteins. Proteins: Structure, Function and Bioinformatics, 2008, 70, 294-299.	2.6	45
57	Protein-protein Docking and Hot-spot Prediction for Drug Discovery. Current Pharmaceutical Design, 2012, 18, 4607-4618.	1.9	41
58	Intermolecular Contact Potentials for Proteinâ€“Protein Interactions Extracted from Binding Free Energy Changes upon Mutation. Journal of Chemical Theory and Computation, 2013, 9, 3715-3727.	5.3	41
59	Prediction and scoring of docking poses with pyDock. Proteins: Structure, Function and Bioinformatics, 2007, 69, 852-858.	2.6	40
60	IRaPPA: information retrieval based integration of biophysical models for protein assembly selection. Bioinformatics, 2017, 33, 1806-1813.	4.1	36
61	STRUCTURAL PREDICTION OF PROTEIN-RNA INTERACTION BY COMPUTATIONAL DOCKING WITH PROPENSITY-BASED STATISTICAL POTENTIALS. , 2009, , 293-301.		33
62	The Long and Short Flavodoxins. Journal of Biological Chemistry, 2004, 279, 47184-47191.	3.4	30
63	EMMPRIN/CD147 is a novel coreceptor of VEGFR-2 mediating its activation by VEGF. Oncotarget, 2015, 6, 9766-9780.	1.8	30
64	Characterizing Changes in the Rate of Protein-Protein Dissociation upon Interface Mutation Using Hotspot Energy and Organization. PLoS Computational Biology, 2013, 9, e1003216.	3.2	29
65	New Efficient Substrates for Semicarbazide-Sensitive Amine Oxidase/VAP-1 Enzyme:â€‰ Analysis by SARs and Computational Docking. Journal of Medicinal Chemistry, 2006, 49, 6197-6208.	6.4	28
66	Structural Basis for Rab1 De-AMPylation by the Legionella pneumophila Effector SidD. PLoS Pathogens, 2013, 9, e1003382.	4.7	28
67	Docking analysis of transient complexes: Interaction of ferredoxinâ€NADP⁺ reductase with ferredoxin and flavodoxin. Proteins: Structure, Function and Bioinformatics, 2008, 72, 848-862.	2.6	26
68	Structural assembly of two-domain proteins by rigid-body docking. BMC Bioinformatics, 2008, 9, 441.	2.6	26
69	Structural characterization of unphosphorylated STAT5a oligomerization equilibrium in solution by smallâ€angle Xâ€ray scattering. Protein Science, 2009, 18, 716-726.	7.6	26
70	Optimization of pyDock for the new CAPRI challenges: Docking of homologyâ€based models, domainâ€“domain assembly and proteinâ€RNA binding. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3182-3188.	2.6	25
71	Mapping of interaction sites of the Schizosaccharomyces pombe protein Translin with nucleic acids and proteins: a combined molecular genetics and bioinformatics study. Nucleic Acids Research, 2010, 38, 2975-2989.	14.5	23
72	Intrinsically active MEK variants are differentially regulated by proteinases and phosphatases. Scientific Reports, 2018, 8, 11830.	3.3	22

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73	Expanding the frontiers of proteinâ€“protein modeling: From docking and scoring to binding affinity predictions and other challenges. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2192-2200.	2.6	20
74	Tetramerizationâ€defects of p53 result in aberrant ubiquitylation and transcriptional activity. Molecular Oncology, 2014, 8, 1026-1042.	4.6	20
75	Helix propensities of conformationally restricted amino acids. Non-natural substitutes for helix breaking proline and helix forming alanine. Organic and Biomolecular Chemistry, 2010, 8, 788.	2.8	19
76	pyDock scoring for the new modeling challenges in docking: Proteinâ€“peptide, homoâ€multimers, and domainâ€“domain interactions. Proteins: Structure, Function and Bioinformatics, 2017, 85, 487-496.	2.6	19
77	Docking approaches for modeling multi-molecular assemblies. Current Opinion in Structural Biology, 2020, 64, 59-65.	5.7	18
78	Apoflavodoxin: Structure, stability, and FMN binding. Biochimie, 1998, 80, 813-820.	2.6	17
79	The 4th meeting on the Critical Assessment of Predicted Interaction (CAPRI) held at the Mare Nostrum, Barcelona. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3065-3066.	2.6	17
80	Structural and Computational Characterization of Disease-Related Mutations Involved in Protein-Protein Interfaces. International Journal of Molecular Sciences, 2019, 20, 1583.	4.1	17
81	Docking-based identification of small-molecule binding sites at protein-protein interfaces. Computational and Structural Biotechnology Journal, 2020, 18, 3750-3761.	4.1	17
82	pyDockCG: New Coarse-Grained Potential for Proteinâ€“Protein Docking. Journal of Physical Chemistry B, 2011, 115, 6032-6039.	2.6	16
83	Structural and energy determinants in protein-RNA docking. Methods, 2017, 118-119, 163-170.	3.8	15
84	pyDockEneRes: per-residue decomposition of proteinâ€“protein docking energy. Bioinformatics, 2020, 36, 2284-2285.	4.1	15
85	The â€˜Relevantâ€™ Stability of Proteins with Equilibrium Intermediates. Scientific World Journal, The, 2002, 2, 1209-1215.	2.1	14
86	Direct interaction between a human digestive protease and the mucoadhesive poly(acrylic acid). Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 784-791.	2.5	14
87	Cell-Dock: high-performance proteinâ€“protein docking. Bioinformatics, 2012, 28, 2394-2396.	4.1	14
88	Intrahelical side chain interactions in Î±-helices: poor correlation between energetics and frequency. FEBS Letters, 1998, 429, 99-103.	2.8	13
89	Docking and scoring: applications to drug discovery in the interactomics era. Expert Opinion on Drug Discovery, 2009, 4, 673-686.	5.0	13
90	Efficient Relaxation of Proteinâ€“Protein Interfaces by Discrete Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 1222-1229.	5.3	13

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91	Inferring the microscopic surface energy of proteinâ€“protein interfaces from mutation data. Proteins: Structure, Function and Bioinformatics, 2015, 83, 640-650.	2.6	13
92	Structural Prediction of Proteinâ€“Protein Interactions by Docking: Application to Biomedical Problems. Advances in Protein Chemistry and Structural Biology, 2018, 110, 203-249.	2.3	13
93	Amino acid residues in the laminin G domains of protein S involved in tissue factor pathway inhibitor interaction. Thrombosis and Haemostasis, 2015, 113, 976-987.	3.4	12
94	A systematic analysis of scoring functions in rigidâ€body protein docking: The delicate balance between the predictive rate improvement and the risk of overtraining. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1287-1297.	2.6	12
95	Protein docking by Rotation-Based Uniform Sampling (RotBUS) with fast computing of intermolecular contact distance and residue desolvation. BMC Bioinformatics, 2010, 11, 352.	2.6	11
96	Conformational transitions in human translin enable nucleic acid binding. Nucleic Acids Research, 2013, 41, 9956-9966.	14.5	11
97	Conformational Heterogeneity of Unbound Proteins Enhances Recognition in Proteinâ€“Protein Encounters. Journal of Chemical Theory and Computation, 2016, 12, 3236-3249.	5.3	11
98	Structural and functional characterization of binding sites in metallocarboxypeptidases based on Optimal Docking Area analysis. Proteins: Structure, Function and Bioinformatics, 2007, 68, 131-144.	2.6	10
99	In silico docking of urokinase plasminogen activator and integrins. BMC Bioinformatics, 2008, 9, S8.	2.6	10
100	Optimization of proteinâ€“protein docking for predicting Fcâ€“protein interactions. Journal of Molecular Recognition, 2016, 29, 555-568.	2.1	10
101	Structural basis for the dominant or recessive character of GLIALCAM mutations found in leukodystrophies. Human Molecular Genetics, 2020, 29, 1107-1120.	2.9	10
102	Docking-based modeling of protein-protein interfaces for extensive structural and functional characterization of missense mutations. PLoS ONE, 2017, 12, e0183643.	2.5	9
103	Computer applications for prediction of protein-protein interactions and rational drug design. Advances and Applications in Bioinformatics and Chemistry, 2009, 2, 101-23.	2.6	9
104	Comment on â€˜proteinâ€“protein binding affinity prediction from amino acid sequenceâ€™. Bioinformatics, 2015, 31, 614-615.	4.1	8
105	Modelling the Evolution of COVID-19 in High-Incidence European Countries and Regions: Estimated Number of Infections and Impact of Past and Future Intervention Measures. Journal of Clinical Medicine, 2020, 9, 1825.	2.4	8
106	New Insights into the Evolution of the Electron Transfer from Cytochrome f to Photosystem I in the Green and Red Branches of Photosynthetic Eukaryotes. Plant and Cell Physiology, 2021, 62, 1082-1093.	3.1	7
107	Structural Characterization of Proteinâ€“Protein Interactions with pyDockSAXS. Methods in Molecular Biology, 2020, 2112, 131-144.	0.9	7
108	Investigation of the diaphorase reaction of ferredoxin-NADP+ reductase by electrochemical methods. Bioelectrochemistry, 1998, 47, 179-183.	1.0	6

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109	Interdomain Conformations in the Full-Length MMP-2 Enzyme Explored by Proteinâ˜Protein Docking Calculations Using pyDock. Journal of Chemical Theory and Computation, 2010, 6, 2204-2213.	5.3	6
110	Integrative modeling of proteinâ€protein interactions with pyDock for the new docking challenges. Proteins: Structure, Function and Bioinformatics, 2020, 88, 999-1008.	2.6	6
111	Substrate specificity of human metallocarboxypeptidase D: Comparison of the two active carboxypeptidase domains. PLoS ONE, 2017, 12, e0187778.	2.5	6
112	Dissection and prediction of RNA-binding sites on proteins. Biomolecular Concepts, 2010, 1, 345-355.	2.2	5
113	Interaction of photosystem I from Phaeodactylum tricornutum with plastocyanins as compared with its native cytochrome c6: Reunion with a lost donor. Biochimica Et Biophysica Acta - Bioenergetics, 2015, 1847, 1549-1559.	1.0	5
114	UEP: an open-source and fast classifier for predicting the impact of mutations in proteinâ€“protein complexes. Bioinformatics, 2021, 37, 334-341.	4.1	5
115	Modeling of Protein Complexes and Molecular Assemblies with pyDock. Methods in Molecular Biology, 2020, 2165, 175-198.	0.9	5
116	Novel treatment strategy for NRAS-mutated melanoma through a selective inhibitor of CD147/VEGFR-2 interaction. Oncogene, 2022, 41, 2254-2264.	5.9	5
117	Docking of cytochrome c6 and plastocyanin to the aa3-type cytochrome c oxidase in the cyanobacterium Phormidium laminosum. Protein Engineering, Design and Selection, 2008, 21, 689-698.	2.1	4
118	Validated Conformational Ensembles Are Key for the Successful Prediction of Protein Complexes. Journal of Chemical Theory and Computation, 2013, 9, 1830-1837.	5.3	4
119	Modeling Binding Affinity of Pathological Mutations for Computational Protein Design. Methods in Molecular Biology, 2017, 1529, 139-159.	0.9	4
120	SCREENED CHARGE ELECTROSTATIC MODEL IN PROTEIN-PROTEIN DOCKING SIMULATIONS. , 2001, , .		4
121	Computer applications for prediction of protein–protein interactions and rational drug design. Advances and Applications in Bioinformatics and Chemistry, 2009, , 101.	2.6	3
122	Predicting protein protein interfaces as clusters of Optimal Docking Area points. International Journal of Data Mining and Bioinformatics, 2009, 3, 55.	0.1	1
123	Unraveling the molecular details of the innate immune response. EBioMedicine, 2016, 9, 7-8.	6.1	1
124	PirePred. Journal of Molecular Diagnostics, 2022, 24, 406-425.	2.8	1
125	Screened charge electrostatic model in protein-protein docking simulations. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2002, , 552-63.	0.7	1
126	Predicting Protein-Protein Interface using Desolvation Energy Similarity Matching. , 2006, , .		0

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127	Editorial. Current Opinion in Structural Biology, 2008, 18, 131-133.	5.7	0
128	Computational Tools for Exploration of the Energy Landscape in Protein-Protein Association. , 2008, , .		0
129	Theory and simulation: integrating models into experimental scenarios. Current Opinion in Structural Biology, 2010, 20, 139-141.	5.7	0
130	Refinement of rigid-body protein–protein docking using backbone and side-chain minimization with a coarse-grained model. Open Access Bioinformatics, 0, , 19.	0.9	0
131	Theory and simulation: complexity and emergence. Current Opinion in Structural Biology, 2012, 22, 127-129.	5.7	0
132	Drug Design on the Cell BE. Chapman & Hall/CRC Computational Science, 2010, , 331-350.	0.5	0