Juan Fernandez-Recio

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4304476/publications.pdf

Version: 2024-02-01

132	6,945	46918 47	71532 76
papers	citations	h-index	g-index

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

#	Article	IF	Citations
1	PirePred. Journal of Molecular Diagnostics, 2022, 24, 406-425.	1.2	1
2	Novel treatment strategy for NRAS-mutated melanoma through a selective inhibitor of CD147/VEGFR-2 interaction. Oncogene, 2022, 41, 2254-2264.	2.6	5
3	UEP: an open-source and fast classifier for predicting the impact of mutations in proteinâ€“protein complexes. Bioinformatics, 2021, 37, 334-341.	1.8	5
4	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.	1.5	7
5	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
6	pyDockEneRes: per-residue decomposition of proteinâ€“protein docking energy. Bioinformatics, 2020, 36, 2284-2285.	1.8	15
7	Integrative modeling of proteinâ€protein interactions with pyDock for the new docking challenges. Proteins: Structure, Function and Bioinformatics, 2020, 88, 999-1008.	1.5	6
8	Docking-based identification of small-molecule binding sites at protein-protein interfaces. Computational and Structural Biotechnology Journal, 2020, 18, 3750-3761.	1.9	17
9	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.	1.0	8
10	Docking approaches for modeling multi-molecular assemblies. Current Opinion in Structural Biology, 2020, 64, 59-65.	2.6	18
11	Structural basis for the dominant or recessive character of GLIALCAM mutations found in leukodystrophies. Human Molecular Genetics, 2020, 29, 1107-1120.	1.4	10
12	Structural Characterization of Proteinâ€“Protein Interactions with pyDockSAXS. Methods in Molecular Biology, 2020, 2112, 131-144.	0.4	7
13	Modeling of Protein Complexes and Molecular Assemblies with pyDock. Methods in Molecular Biology, 2020, 2165, 175-198.	0.4	5
14	SKEMPI 2.0: an updated benchmark of changes in proteinâ€“protein binding energy, kinetics and thermodynamics upon mutation. Bioinformatics, 2019, 35, 462-469.	1.8	191
15	Blind prediction of homoâ€and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	1.5	99
16	L amino acid transporter structure and molecular bases for the asymmetry of substrate interaction. Nature Communications, 2019, 10, 1807.	5.8	57
17	Structural and Computational Characterization of Disease-Related Mutations Involved in Protein-Protein Interfaces. International Journal of Molecular Sciences, 2019, 20, 1583.	1.8	17
18	Hot-spot analysis for drug discovery targeting protein-protein interactions. Expert Opinion on Drug Discovery, 2018, 13, 327-338.	2.5	64

#	Article	IF	Citations
19	LightDock: a new multi-scale approach to proteinâ€“protein docking. Bioinformatics, 2018, 34, 49-55.	1.8	83
20	Structural Prediction of Proteinâ€“Protein Interactions by Docking: Application to Biomedical Problems. Advances in Protein Chemistry and Structural Biology, 2018, 110, 203-249.	1.0	13
21	Intrinsically active MEK variants are differentially regulated by proteinases and phosphatases. Scientific Reports, 2018, 8, 11830.	1.6	22
22	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.	1.5	12
23	Modeling Binding Affinity of Pathological Mutations for Computational Protein Design. Methods in Molecular Biology, 2017, 1529, 139-159.	0.4	4
24	Structural and energy determinants in protein-RNA docking. Methods, 2017, 118-119, 163-170.	1.9	15
25	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.	1.5	19
26	IRaPPA: information retrieval based integration of biophysical models for protein assembly selection. Bioinformatics, 2017, 33, 1806-1813.	1.8	36
27	Docking-based modeling of protein-protein interfaces for extensive structural and functional characterization of missense mutations. PLoS ONE, 2017, 12, e0183643.	1.1	9
28	Substrate specificity of human metallocarboxypeptidase D: Comparison of the two active carboxypeptidase domains. PLoS ONE, 2017, 12, e0187778.	1.1	6
29	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
30	Unraveling the molecular details of the innate immune response. EBioMedicine, 2016, 9, 7-8.	2.7	1
31	Optimization of proteinâ€“protein docking for predicting Fcâ€“protein interactions. Journal of Molecular Recognition, 2016, 29, 555-568.	1.1	10
32	Conformational Heterogeneity of Unbound Proteins Enhances Recognition in Proteinâ€“Protein Encounters. Journal of Chemical Theory and Computation, 2016, 12, 3236-3249.	2.3	11
33	Inferring the microscopic surface energy of proteinâ€“protein interfaces from mutation data. Proteins: Structure, Function and Bioinformatics, 2015, 83, 640-650.	1.5	13
34	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.	1.8	12
35	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.	0.5	5
36	pyDockSAXS: proteinâ€“protein complex structure by SAXS and computational docking. Nucleic Acids Research, 2015, 43, W356-W361.	6.5	61

#	Article	IF	Citations
37	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
38	Comment on â€˜proteinâ€“protein binding affinity prediction from amino acid sequenceâ€™. Bioinformatics, 2015, 31, 614-615.	1.8	8
39	CCharPPI web server: computational characterization of proteinâ€“protein interactions from structure. Bioinformatics, 2015, 31, 123-125.	1.8	61
40	EMMPRIN/CD147 is a novel coreceptor of VEGFR-2 mediating its activation by VEGF. Oncotarget, 2015, 6, 9766-9780.	0.8	30
41	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.	3.3	84
42	Tetramerizationâ€defects of p53 result in aberrant ubiquitylation and transcriptional activity. Molecular Oncology, 2014, 8, 1026-1042.	2.1	20
43	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	1.5	50
44	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.	3.3	46
45	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.	1.5	20
46	Scoring functions for proteinâ€“protein interactions. Current Opinion in Structural Biology, 2013, 23, 862-867.	2.6	87
47	pyDockWEB: a web server for rigid-body proteinâ€“protein docking using electrostatics and desolvation scoring. Bioinformatics, 2013, 29, 1698-1699.	1.8	214
48	SwarmDock: a server for flexible proteinâ€“protein docking. Bioinformatics, 2013, 29, 807-809.	1.8	259
49	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.	2.3	41
50	The scoring of poses in protein-protein docking: current capabilities and future directions. BMC Bioinformatics, 2013, 14, 286.	1.2	98
51	Efficient Relaxation of Proteinâ€“Protein Interfaces by Discrete Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 1222-1229.	2.3	13
52	Validated Conformational Ensembles Are Key for the Successful Prediction of Protein Complexes. Journal of Chemical Theory and Computation, 2013, 9, 1830-1837.	2.3	4
53	Characterizing Changes in the Rate of Protein-Protein Dissociation upon Interface Mutation Using Hotspot Energy and Organization. PLoS Computational Biology, 2013, 9, e1003216.	1.5	29
54	Structural Basis for Rab1 De-AMPylation by the Legionella pneumophila Effector SidD. PLoS Pathogens, 2013, 9, e1003382.	2.1	28

#	Article	IF	Citations
55	Conformational transitions in human translin enable nucleic acid binding. Nucleic Acids Research, 2013, 41, 9956-9966.	6.5	11
56	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
57	SKEMPI: a Structural Kinetic and Energetic database of Mutant Protein Interactions and its use in empirical models. Bioinformatics, 2012, 28, 2600-2607.	1.8	237
58	Cell-Dock: high-performance proteinâ€“protein docking. Bioinformatics, 2012, 28, 2394-2396.	1.8	14
59	Protein-protein Docking and Hot-spot Prediction for Drug Discovery. Current Pharmaceutical Design, 2012, 18, 4607-4618.	0.9	41
60	A proteinâ€RNA docking benchmark (II): Extended set from experimental and homology modeling data. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1872-1882.	1.5	46
61	Allosteric Conversation in the Androgen Receptor Ligand-Binding Domain Surfaces. Molecular Endocrinology, 2012, 26, 1078-1090.	3.7	58
62	Established and Emerging Trends in Computational Drug Discovery in the Structural Genomics Era. Chemistry and Biology, 2012, 19, 29-41.	6.2	57
63	Theory and simulation: complexity and emergence. Current Opinion in Structural Biology, 2012, 22, 127-129.	2.6	0
64	pyDockCG: New Coarse-Grained Potential for Proteinâ€“Protein Docking. Journal of Physical Chemistry B, 2011, 115, 6032-6039.	1.2	16
65	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.	2.5	70
66	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	2.0	131
67	LRR Conservation Mapping to Predict Functional Sites within Protein Leucine-Rich Repeat Domains. PLoS ONE, 2011, 6, e21614.	1.1	46
68	Prediction of protein binding sites and hot spots. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 680-698.	6.2	50
69	Prediction of protein-binding areas by small-world residue networks and application to docking. BMC Bioinformatics, 2011, 12, 378.	1.2	46
70	Theory and simulation: integrating models into experimental scenarios. Current Opinion in Structural Biology, 2010, 20, 139-141.	2.6	0
71	Protein docking by Rotation-Based Uniform Sampling (RotBUS) with fast computing of intermolecular contact distance and residue desolvation. BMC Bioinformatics, 2010, 11, 352.	1.2	11
72	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.	1.5	83

#	Article	IF	Citations
73	Present and future challenges and limitations in proteinâ€“protein docking. Proteins: Structure, Function and Bioinformatics, 2010, 78, 95-108.	1.5	76
74	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.	1.5	25
75	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.	1.5	17
76	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.	6.5	23
77	Dissection and prediction of RNA-binding sites on proteins. Biomolecular Concepts, 2010, 1, 345-355.	1.0	5
78	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.	2.3	6
79	Structural Characterization of Proteinâ€“Protein Complexes by Integrating Computational Docking with Small-angle Scattering Data. Journal of Molecular Biology, 2010, 403, 217-230.	2.0	64
80	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.	1.5	19
81	Drug Design on the Cell BE. Chapman & Hall/CRC Computational Science, 2010, , 331-350.	0.5	0
82	Computer applications for prediction of protein–protein interactions and rational drug design. Advances and Applications in Bioinformatics and Chemistry, 2009, , 101.	1.6	3
83	STRUCTURAL PREDICTION OF PROTEIN-RNA INTERACTION BY COMPUTATIONAL DOCKING WITH PROPENSITY-BASED STATISTICAL POTENTIALS. , 2009, , 293-301.		33
84	Pushing Structural Information into the Yeast Interactome by High-Throughput Protein Docking Experiments. PLoS Computational Biology, 2009, 5, e1000490.	1.5	67
85	FRODOCK: a new approach for fast rotational proteinâ€“protein docking. Bioinformatics, 2009, 25, 2544-2551.	1.8	126
86	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.	3.3	68
87	Structural characterization of unphosphorylated STAT5a oligomerization equilibrium in solution by smallâ€angle Xâ€ray scattering. Protein Science, 2009, 18, 716-726.	3.1	26
88	Soft protein-protein docking in internal coordinates. Protein Science, 2009, 11, 280-291.	3.1	175
89	Docking and scoring: applications to drug discovery in the interactomics era. Expert Opinion on Drug Discovery, 2009, 4, 673-686.	2.5	13
90	Predicting protein protein interfaces as clusters of Optimal Docking Area points. International Journal of Data Mining and Bioinformatics, 2009, 3, 55.	0.1	1

#	Article	IF	Citations
91	Computer applications for prediction of protein-protein interactions and rational drug design. Advances and Applications in Bioinformatics and Chemistry, 2009, 2, 101-23.	1.6	9
92	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.	1.5	45
93	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
94	Docking analysis of transient complexes: Interaction of ferredoxinâ€NADP⁺ reductase with ferredoxin and flavodoxin. Proteins: Structure, Function and Bioinformatics, 2008, 72, 848-862.	1.5	26
95	Structural assembly of two-domain proteins by rigid-body docking. BMC Bioinformatics, 2008, 9, 441.	1.2	26
96	Identification of hot-spot residues in protein-protein interactions by computational docking. BMC Bioinformatics, 2008, 9, 447.	1.2	107
97	In silico docking of urokinase plasminogen activator and integrins. BMC Bioinformatics, 2008, 9, S8.	1.2	10
98	Editorial. Current Opinion in Structural Biology, 2008, 18, 131-133.	2.6	0
99	Assembly and Channel Opening in a Bacterial Drug Efflux Machine. Molecular Cell, 2008, 30, 114-121.	4.5	155
100	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.	1.0	4
101	Computational Tools for Exploration of the Energy Landscape in Protein-Protein Association. , 2008, , .		0
102	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.	1.6	101
103	Recognition and Cooperation Between the ATP-dependent RNA Helicase RhlB and Ribonuclease RNase E. Journal of Molecular Biology, 2007, 367, 113-132.	2.0	66
104	Structural and functional characterization of binding sites in metallocarboxypeptidases based on Optimal Docking Area analysis. Proteins: Structure, Function and Bioinformatics, 2007, 68, 131-144.	1.5	10
105	pyDock: Electrostatics and desolvation for effective scoring of rigid-body protein-protein docking. Proteins: Structure, Function and Bioinformatics, 2007, 68, 503-515.	1.5	286
106	Prediction and scoring of docking poses with pyDock. Proteins: Structure, Function and Bioinformatics, 2007, 69, 852-858.	1.5	40
107	Predicting Protein-Protein Interface using Desolvation Energy Similarity Matching. , 2006, , .		0
108	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.	2.9	28

#	Article	IF	Citations
109	The Crystal Structure of the BAR Domain from Human Bin1/Amphiphysin II and Its Implications for Molecular Recognitionâ€. Biochemistry, 2006, 45, 12917-12928.	1.2	72
110	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.	2.0	58
111	Polygalacturonase inhibiting proteins: players in plant innate immunity?. Trends in Plant Science, 2006, 11, 65-70.	4.3	153
112	Brief encounters bolster contacts. Nature, 2006, 444, 279-280.	13.7	46
113	Identifying interaction motifs in CK2Î² â€“ a ubiquitous kinase regulatory subunit. Trends in Biochemical Sciences, 2006, 31, 654-661.	3.7	51
114	Improving CAPRI predictions: Optimized desolvation for rigid-body docking. Proteins: Structure, Function and Bioinformatics, 2005, 60, 308-313.	1.5	45
115	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.	2.3	53
116	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.	1.6	91
117	The Long and Short Flavodoxins. Journal of Biological Chemistry, 2004, 279, 47184-47191.	1.6	30
118	Optimal docking area: A new method for predicting protein-protein interaction sites. Proteins: Structure, Function and Bioinformatics, 2004, 58, 134-143.	1.5	185
119	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.	1.2	116
120	A model of a transmembrane drug-efflux pump from Gram-negative bacteria. FEBS Letters, 2004, 578, 5-9.	1.3	71
121	Identification of Proteinâ€“Protein Interaction Sites from Docking Energy Landscapes. Journal of Molecular Biology, 2004, 335, 843-865.	2.0	276
122	ICM-DISCO docking by global energy optimization with fully flexible side-chains. Proteins: Structure, Function and Bioinformatics, 2003, 52, 113-117.	1.5	183
123	The â€˜Relevantâ€™ Stability of Proteins with Equilibrium Intermediates. Scientific World Journal, The, 2002, 2, 1209-1215.	0.8	14
124	Screened charge electrostatic model in protein-protein docking simulations. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2002, , 552-63.	0.7	1
125	SCREENED CHARGE ELECTROSTATIC MODEL IN PROTEIN-PROTEIN DOCKING SIMULATIONS. , 2001, , .		4
126	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.	6.6	63

#	Article	IF	Citations
127	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.	2.0	73
128	Investigation of the diaphorase reaction of ferredoxin-NADP+ reductase by electrochemical methods. Bioelectrochemistry, 1998, 47, 179-183.	1.0	6
129	Apoflavodoxin: Structure, stability, and FMN binding. Biochimie, 1998, 80, 813-820.	1.3	17
130	Intrahelical side chain interactions in Î±-helices: poor correlation between energetics and frequency. FEBS Letters, 1998, 429, 99-103.	1.3	13
131	The Tryptophan/Histidine interaction in Î±-helices. Journal of Molecular Biology, 1997, 267, 184-197.	2.0	101
132	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