

Juan Fernandez-Recio

List of Publications by Year in descending order

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132
papers

6,945
citations

47006

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h-index

71685

76
g-index

140
all docs

140
docs citations

140
times ranked

6929
citing authors

#	ARTICLE	IF	CITATIONS
1	PirePred. Journal of Molecular Diagnostics, 2022, 24, 406-425.	2.8	1
2	Novel treatment strategy for NRAS-mutated melanoma through a selective inhibitor of CD147/VEGFR-2 interaction. Oncogene, 2022, 41, 2254-2264.	5.9	5
3	UEP: an open-source and fast classifier for predicting the impact of mutations in protein-protein complexes. Bioinformatics, 2021, 37, 334-341.	4.1	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.	3.1	7
5	Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1800-1823.	2.6	73
6	pyDockEneRes: per-residue decomposition of protein-protein docking energy. Bioinformatics, 2020, 36, 2284-2285.	4.1	15
7	Integrative modeling of protein-protein interactions with pyDock for the new docking challenges. Proteins: Structure, Function and Bioinformatics, 2020, 88, 999-1008.	2.6	6
8	Docking-based identification of small-molecule binding sites at protein-protein interfaces. Computational and Structural Biotechnology Journal, 2020, 18, 3750-3761.	4.1	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.	2.4	8
10	Docking approaches for modeling multi-molecular assemblies. Current Opinion in Structural Biology, 2020, 64, 59-65.	5.7	18
11	Structural basis for the dominant or recessive character of GLIALCAM mutations found in leukodystrophies. Human Molecular Genetics, 2020, 29, 1107-1120.	2.9	10
12	Structural Characterization of Protein-Protein Interactions with pyDockSAXS. Methods in Molecular Biology, 2020, 2112, 131-144.	0.9	7
13	Modeling of Protein Complexes and Molecular Assemblies with pyDock. Methods in Molecular Biology, 2020, 2165, 175-198.	0.9	5
14	SKEMPI 2.0: an updated benchmark of changes in protein-protein binding energy, kinetics and thermodynamics upon mutation. Bioinformatics, 2019, 35, 462-469.	4.1	191
15	Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	2.6	99
16	L amino acid transporter structure and molecular bases for the asymmetry of substrate interaction. Nature Communications, 2019, 10, 1807.	12.8	57
17	Structural and Computational Characterization of Disease-Related Mutations Involved in Protein-Protein Interfaces. International Journal of Molecular Sciences, 2019, 20, 1583.	4.1	17
18	Hot-spot analysis for drug discovery targeting protein-protein interactions. Expert Opinion on Drug Discovery, 2018, 13, 327-338.	5.0	64

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19	LightDock: a new multi-scale approach to protein-protein docking. <i>Bioinformatics</i> , 2018, 34, 49-55.	4.1	83
20	Structural Prediction of Protein-Protein Interactions by Docking: Application to Biomedical Problems. <i>Advances in Protein Chemistry and Structural Biology</i> , 2018, 110, 203-249.	2.3	13
21	Intrinsically active MEK variants are differentially regulated by proteinases and phosphatases. <i>Scientific Reports</i> , 2018, 8, 11830.	3.3	22
22	A systematic analysis of scoring functions in rigid-body protein docking: The delicate balance between the predictive rate improvement and the risk of overtraining. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1287-1297.	2.6	12
23	Modeling Binding Affinity of Pathological Mutations for Computational Protein Design. <i>Methods in Molecular Biology</i> , 2017, 1529, 139-159.	0.9	4
24	Structural and energy determinants in protein-RNA docking. <i>Methods</i> , 2017, 118-119, 163-170.	3.8	15
25	pyDock scoring for the new modeling challenges in docking: Protein-peptide, homo-multimers, and domain-domain interactions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 487-496.	2.6	19
26	IRaPPA: information retrieval based integration of biophysical models for protein assembly selection. <i>Bioinformatics</i> , 2017, 33, 1806-1813.	4.1	36
27	Docking-based modeling of protein-protein interfaces for extensive structural and functional characterization of missense mutations. <i>PLoS ONE</i> , 2017, 12, e0183643.	2.5	9
28	Substrate specificity of human metallopeptidase D: Comparison of the two active carboxypeptidase domains. <i>PLoS ONE</i> , 2017, 12, e0187778.	2.5	6
29	Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 323-348.	2.6	148
30	Unraveling the molecular details of the innate immune response. <i>EBioMedicine</i> , 2016, 9, 7-8.	6.1	1
31	Optimization of protein-protein docking for predicting Fc-protein interactions. <i>Journal of Molecular Recognition</i> , 2016, 29, 555-568.	2.1	10
32	Conformational Heterogeneity of Unbound Proteins Enhances Recognition in Protein-Protein Encounters. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3236-3249.	5.3	11
33	Inferring the microscopic surface energy of protein-protein interfaces from mutation data. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 640-650.	2.6	13
34	Amino acid residues in the laminin G domains of protein S involved in tissue factor pathway inhibitor interaction. <i>Thrombosis and Haemostasis</i> , 2015, 113, 976-987.	3.4	12
35	Interaction of photosystem I from <i>Phaeodactylum tricornutum</i> with plastocyanins as compared with its native cytochrome c6: Reunion with a lost donor. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2015, 1847, 1549-1559.	1.0	5
36	pyDockSAXS: protein-protein complex structure by SAXS and computational docking. <i>Nucleic Acids Research</i> , 2015, 43, W356-W361.	14.5	61

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37	Updates to the Integrated Protein-Protein Interaction Benchmarks: Docking Benchmark Version 5 and Affinity Benchmark Version 2. <i>Journal of Molecular Biology</i> , 2015, 427, 3031-3041.	4.2	348
38	Comment on "protein-protein binding affinity prediction from amino acid sequence". <i>Bioinformatics</i> , 2015, 31, 614-615.	4.1	8
39	CCharPPI web server: computational characterization of protein-protein interactions from structure. <i>Bioinformatics</i> , 2015, 31, 123-125.	4.1	61
40	EMMPRIN/CD147 is a novel coreceptor of VEGFR-2 mediating its activation by VEGF. <i>Oncotarget</i> , 2015, 6, 9766-9780.	1.8	30
41	Structural bases for the interaction and stabilization of the human amino acid transporter LAT2 with its ancillary protein 4F2hc. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 2966-2971.	7.1	84
42	Tetramerization-defects of p53 result in aberrant ubiquitylation and transcriptional activity. <i>Molecular Oncology</i> , 2014, 8, 1026-1042.	4.6	20
43	Blind prediction of interfacial water positions in CAPRI. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 620-632.	2.6	50
44	Structural basis for the recruitment and activation of the <i>Legionella</i> phospholipase VipD by the host GTPase Rab5. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, E3514-23.	7.1	46
45	Expanding the frontiers of protein-protein modeling: From docking and scoring to binding affinity predictions and other challenges. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 2192-2200.	2.6	20
46	Scoring functions for protein-protein interactions. <i>Current Opinion in Structural Biology</i> , 2013, 23, 862-867.	5.7	87
47	pyDockWEB: a web server for rigid-body protein-protein docking using electrostatics and desolvation scoring. <i>Bioinformatics</i> , 2013, 29, 1698-1699.	4.1	214
48	SwarmDock: a server for flexible protein-protein docking. <i>Bioinformatics</i> , 2013, 29, 807-809.	4.1	259
49	Intermolecular Contact Potentials for Protein-Protein Interactions Extracted from Binding Free Energy Changes upon Mutation. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3715-3727.	5.3	41
50	The scoring of poses in protein-protein docking: current capabilities and future directions. <i>BMC Bioinformatics</i> , 2013, 14, 286.	2.6	98
51	Efficient Relaxation of Protein-Protein Interfaces by Discrete Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1222-1229.	5.3	13
52	Validated Conformational Ensembles Are Key for the Successful Prediction of Protein Complexes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1830-1837.	5.3	4
53	Characterizing Changes in the Rate of Protein-Protein Dissociation upon Interface Mutation Using Hotspot Energy and Organization. <i>PLoS Computational Biology</i> , 2013, 9, e1003216.	3.2	29
54	Structural Basis for Rab1 De-AMPylation by the <i>Legionella pneumophila</i> Effector SidD. <i>PLoS Pathogens</i> , 2013, 9, e1003382.	4.7	28

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55	Conformational transitions in human translin enable nucleic acid binding. <i>Nucleic Acids Research</i> , 2013, 41, 9956-9966.	14.5	11
56	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 1980-1987.	2.6	87
57	SKEMPI: a Structural Kinetic and Energetic database of Mutant Protein Interactions and its use in empirical models. <i>Bioinformatics</i> , 2012, 28, 2600-2607.	4.1	237
58	Cell-Dock: high-performance protein-protein docking. <i>Bioinformatics</i> , 2012, 28, 2394-2396.	4.1	14
59	Protein-protein Docking and Hot-spot Prediction for Drug Discovery. <i>Current Pharmaceutical Design</i> , 2012, 18, 4607-4618.	1.9	41
60	A protein-RNA docking benchmark (II): Extended set from experimental and homology modeling data. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 1872-1882.	2.6	46
61	Allosteric Conversation in the Androgen Receptor Ligand-Binding Domain Surfaces. <i>Molecular Endocrinology</i> , 2012, 26, 1078-1090.	3.7	58
62	Established and Emerging Trends in Computational Drug Discovery in the Structural Genomics Era. <i>Chemistry and Biology</i> , 2012, 19, 29-41.	6.0	57
63	Theory and simulation: complexity and emergence. <i>Current Opinion in Structural Biology</i> , 2012, 22, 127-129.	5.7	0
64	pyDockCG: New Coarse-Grained Potential for Protein-Protein Docking. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6032-6039.	2.6	16
65	Scoring by Intermolecular Pairwise Propensities of Exposed Residues (SIPPER): A New Efficient Potential for Protein-Protein Docking. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 370-377.	5.4	70
66	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. <i>Journal of Molecular Biology</i> , 2011, 414, 289-302.	4.2	131
67	LRR Conservation Mapping to Predict Functional Sites within Protein Leucine-Rich Repeat Domains. <i>PLoS ONE</i> , 2011, 6, e21614.	2.5	46
68	Prediction of protein binding sites and hot spots. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 680-698.	14.6	50
69	Prediction of protein-binding areas by small-world residue networks and application to docking. <i>BMC Bioinformatics</i> , 2011, 12, 378.	2.6	46
70	Theory and simulation: integrating models into experimental scenarios. <i>Current Opinion in Structural Biology</i> , 2010, 20, 139-141.	5.7	0
71	Protein docking by Rotation-Based Uniform Sampling (RotBUS) with fast computing of intermolecular contact distance and residue desolvation. <i>BMC Bioinformatics</i> , 2010, 11, 352.	2.6	11
72	Optimal protein-RNA area, OPRA: A propensity-based method to identify RNA-binding sites on proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 25-35.	2.6	83

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73	Present and future challenges and limitations in protein-protein docking. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 95-108.	2.6	76
74	Optimization of pyDock for the new CAPRI challenges: Docking of homology-based models, domain-domain assembly and protein-RNA binding. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 3182-3188.	2.6	25
75	The 4th meeting on the Critical Assessment of Predicted Interaction (CAPRI) held at the Mare Nostrum, Barcelona. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 3065-3066.	2.6	17
76	Mapping of interaction sites of the <i>Schizosaccharomyces pombe</i> protein Translin with nucleic acids and proteins: a combined molecular genetics and bioinformatics study. <i>Nucleic Acids Research</i> , 2010, 38, 2975-2989.	14.5	23
77	Dissection and prediction of RNA-binding sites on proteins. <i>Biomolecular Concepts</i> , 2010, 1, 345-355.	2.2	5
78	Interdomain Conformations in the Full-Length MMP-2 Enzyme Explored by Protein-Protein Docking Calculations Using pyDock. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2204-2213.	5.3	6
79	Structural Characterization of Protein-Protein Complexes by Integrating Computational Docking with Small-angle Scattering Data. <i>Journal of Molecular Biology</i> , 2010, 403, 217-230.	4.2	64
80	Helix propensities of conformationally restricted amino acids. Non-natural substitutes for helix breaking proline and helix forming alanine. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 788.	2.8	19
81	Drug Design on the Cell BE. <i>Chapman & Hall/CRC Computational Science</i> , 2010, , 331-350.	0.5	0
82	Computer applications for prediction of protein-protein interactions and rational drug design. <i>Advances and Applications in Bioinformatics and Chemistry</i> , 2009, , 101.	2.6	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. <i>PLoS Computational Biology</i> , 2009, 5, e1000490.	3.2	67
85	FRODOCK: a new approach for fast rotational protein-protein docking. <i>Bioinformatics</i> , 2009, 25, 2544-2551.	4.1	126
86	Integration of evolutionary and desolvation energy analysis identifies functional sites in a plant immunity protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 7666-7671.	7.1	68
87	Structural characterization of unphosphorylated STAT5a oligomerization equilibrium in solution by small-angle X-ray scattering. <i>Protein Science</i> , 2009, 18, 716-726.	7.6	26
88	Soft protein-protein docking in internal coordinates. <i>Protein Science</i> , 2009, 11, 280-291.	7.6	175
89	Docking and scoring: applications to drug discovery in the interactomics era. <i>Expert Opinion on Drug Discovery</i> , 2009, 4, 673-686.	5.0	13
90	Predicting protein protein interfaces as clusters of Optimal Docking Area points. <i>International Journal of Data Mining and Bioinformatics</i> , 2009, 3, 55.	0.1	1

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91	Computer applications for prediction of protein-protein interactions and rational drug design. <i>Advances and Applications in Bioinformatics and Chemistry</i> , 2009, 2, 101-23.	2.6	9
92	Crystal structure of the endopolygalacturonase from the phytopathogenic fungus <i>Colletotrichum lupini</i> and its interaction with polygalacturonase-inhibiting proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 294-299.	2.6	45
93	Direct interaction between a human digestive protease and the mucoadhesive poly(acrylic acid). <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2008, 64, 784-791.	2.5	14
94	Docking analysis of transient complexes: Interaction of ferredoxin-NADP ⁺ reductase with ferredoxin and flavodoxin. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 72, 848-862.	2.6	26
95	Structural assembly of two-domain proteins by rigid-body docking. <i>BMC Bioinformatics</i> , 2008, 9, 441.	2.6	26
96	Identification of hot-spot residues in protein-protein interactions by computational docking. <i>BMC Bioinformatics</i> , 2008, 9, 447.	2.6	107
97	In silico docking of urokinase plasminogen activator and integrins. <i>BMC Bioinformatics</i> , 2008, 9, S8.	2.6	10
98	Editorial. <i>Current Opinion in Structural Biology</i> , 2008, 18, 131-133.	5.7	0
99	Assembly and Channel Opening in a Bacterial Drug Efflux Machine. <i>Molecular Cell</i> , 2008, 30, 114-121.	9.7	155
100	Docking of cytochrome c6 and plastocyanin to the aa3-type cytochrome c oxidase in the cyanobacterium <i>Phormidium laminosum</i> . <i>Protein Engineering, Design and Selection</i> , 2008, 21, 689-698.	2.1	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. <i>Journal of Biological Chemistry</i> , 2007, 282, 31444-31452.	3.4	101
103	Recognition and Cooperation Between the ATP-dependent RNA Helicase RhlB and Ribonuclease RNase E. <i>Journal of Molecular Biology</i> , 2007, 367, 113-132.	4.2	66
104	Structural and functional characterization of binding sites in metallo-carboxypeptidases based on Optimal Docking Area analysis. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 68, 131-144.	2.6	10
105	pyDock: Electrostatics and desolvation for effective scoring of rigid-body protein-protein docking. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 68, 503-515.	2.6	286
106	Prediction and scoring of docking poses with pyDock. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 69, 852-858.	2.6	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: Analysis by SARs and Computational Docking. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 6197-6208.	6.4	28

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109	The Crystal Structure of the BAR Domain from Human Bin1/Amphiphysin II and Its Implications for Molecular Recognition. <i>Biochemistry</i> , 2006, 45, 12917-12928.	2.5	72
110	Efficient Restraints for Protein-Protein Docking by Comparison of Observed Amino Acid Substitution Patterns with those Predicted from Local Environment. <i>Journal of Molecular Biology</i> , 2006, 357, 1669-1682.	4.2	58
111	Polygalacturonase inhibiting proteins: players in plant innate immunity?. <i>Trends in Plant Science</i> , 2006, 11, 65-70.	8.8	153
112	Brief encounters bolster contacts. <i>Nature</i> , 2006, 444, 279-280.	27.8	46
113	Identifying interaction motifs in CK2 β - a ubiquitous kinase regulatory subunit. <i>Trends in Biochemical Sciences</i> , 2006, 31, 654-661.	7.5	51
114	Improving CAPRI predictions: Optimized desolvation for rigid-body docking. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 60, 308-313.	2.6	45
115	The Polygalacturonase-Inhibiting Protein PGIP2 of <i>Phaseolus vulgaris</i> Has Evolved a Mixed Mode of Inhibition of Endopolygalacturonase PG1 of <i>Botrytis cinerea</i> . <i>Plant Physiology</i> , 2005, 139, 1380-1388.	4.8	53
116	The Crystal Structure of the Outer Membrane Protein VceC from the Bacterial Pathogen <i>Vibrio cholerae</i> at 1.8 Å... Resolution. <i>Journal of Biological Chemistry</i> , 2005, 280, 15307-15314.	3.4	91
117	The Long and Short Flavodoxins. <i>Journal of Biological Chemistry</i> , 2004, 279, 47184-47191.	3.4	30
118	Optimal docking area: A new method for predicting protein-protein interaction sites. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 58, 134-143.	2.6	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 Affinity. <i>Biochemistry</i> , 2004, 43, 629-640.	2.5	116
120	A model of a transmembrane drug-efflux pump from Gram-negative bacteria. <i>FEBS Letters</i> , 2004, 578, 5-9.	2.8	71
121	Identification of Protein-Protein Interaction Sites from Docking Energy Landscapes. <i>Journal of Molecular Biology</i> , 2004, 335, 843-865.	4.2	276
122	ICM-DISCO docking by global energy optimization with fully flexible side-chains. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 52, 113-117.	2.6	183
123	The "Relevant"™ Stability of Proteins with Equilibrium Intermediates. <i>Scientific World Journal</i> , The, 2002, 2, 1209-1215.	2.1	14
124	Screened charge electrostatic model in protein-protein docking simulations. <i>Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing</i> , 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. <i>Journal of the American Chemical Society</i> , 2000, 122, 9808-9817.	13.7	63

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127	Energetics of a hydrogen bond (charged and neutral) and of a cation- π interaction in apoflavodoxin 1 Edited by A. R. Fersht. Journal of Molecular Biology, 1999, 290, 319-330.	4.2	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.	2.6	17
130	Intrahelical side chain interactions in α -helices: poor correlation between energetics and frequency. FEBS Letters, 1998, 429, 99-103.	2.8	13
131	The Tryptophan/Histidine interaction in α -helices. Journal of Molecular Biology, 1997, 267, 184-197.	4.2	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