

Juan Fernandez-Recio

List of Publications by Year in descending order

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132
papers

6,945
citations

46918

47
h-index

71532

76
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140
all docs

140
docs citations

140
times ranked

6929
citing authors

#	ARTICLE	IF	CITATIONS
1	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.	2.0	348
2	pyDock: Electrostatics and desolvation for effective scoring of rigid-body protein-protein docking. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 68, 503-515.	1.5	286
3	Identification of Protein-Protein Interaction Sites from Docking Energy Landscapes. <i>Journal of Molecular Biology</i> , 2004, 335, 843-865.	2.0	276
4	SwarmDock: a server for flexible protein-protein docking. <i>Bioinformatics</i> , 2013, 29, 807-809.	1.8	259
5	SKEMPI: a Structural Kinetic and Energetic database of Mutant Protein Interactions and its use in empirical models. <i>Bioinformatics</i> , 2012, 28, 2600-2607.	1.8	237
6	pyDockWEB: a web server for rigid-body protein-protein docking using electrostatics and desolvation scoring. <i>Bioinformatics</i> , 2013, 29, 1698-1699.	1.8	214
7	SKEMPI 2.0: an updated benchmark of changes in protein-protein binding energy, kinetics and thermodynamics upon mutation. <i>Bioinformatics</i> , 2019, 35, 462-469.	1.8	191
8	Optimal docking area: A new method for predicting protein-protein interaction sites. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 58, 134-143.	1.5	185
9	ICM-DISCO docking by global energy optimization with fully flexible side-chains. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 52, 113-117.	1.5	183
10	Soft protein-protein docking in internal coordinates. <i>Protein Science</i> , 2009, 11, 280-291.	3.1	175
11	Assembly and Channel Opening in a Bacterial Drug Efflux Machine. <i>Molecular Cell</i> , 2008, 30, 114-121.	4.5	155
12	Polygalacturonase inhibiting proteins: players in plant innate immunity?. <i>Trends in Plant Science</i> , 2006, 11, 65-70.	4.3	153
13	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.	1.5	148
14	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. <i>Journal of Molecular Biology</i> , 2011, 414, 289-302.	2.0	131
15	FRODOCK: a new approach for fast rotational protein-protein docking. <i>Bioinformatics</i> , 2009, 25, 2544-2551.	1.8	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 Affinity. <i>Biochemistry</i> , 2004, 43, 629-640.	1.2	116
17	Identification of hot-spot residues in protein-protein interactions by computational docking. <i>BMC Bioinformatics</i> , 2008, 9, 447.	1.2	107
18	The Tryptophan/Histidine interaction in α -helices. <i>Journal of Molecular Biology</i> , 1997, 267, 184-197.	2.0	101

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19	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.	1.6	101
20	Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 1200-1221.	1.5	99
21	The scoring of poses in protein-protein docking: current capabilities and future directions. <i>BMC Bioinformatics</i> , 2013, 14, 286.	1.2	98
22	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.	1.6	91
23	Scoring functions for protein-protein interactions. <i>Current Opinion in Structural Biology</i> , 2013, 23, 862-867.	2.6	87
24	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.	1.5	87
25	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.	3.3	84
26	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.	1.5	83
27	LightDock: a new multi-scale approach to protein-protein docking. <i>Bioinformatics</i> , 2018, 34, 49-55.	1.8	83
28	Present and future challenges and limitations in protein-protein docking. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 95-108.	1.5	76
29	Energetics of a hydrogen bond (charged and neutral) and of a cation-π interaction in apoflavodoxin 1 Edited by A. R. Fersht. <i>Journal of Molecular Biology</i> , 1999, 290, 319-330.	2.0	73
30	Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 1800-1823.	1.5	73
31	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.	1.2	72
32	A model of a transmembrane drug-efflux pump from Gram-negative bacteria. <i>FEBS Letters</i> , 2004, 578, 5-9.	1.3	71
33	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.	2.5	70
34	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.	3.3	68
35	Pushing Structural Information into the Yeast Interactome by High-Throughput Protein Docking Experiments. <i>PLoS Computational Biology</i> , 2009, 5, e1000490.	1.5	67
36	Recognition and Cooperation Between the ATP-dependent RNA Helicase RhlB and Ribonuclease RNase E. <i>Journal of Molecular Biology</i> , 2007, 367, 113-132.	2.0	66

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37	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.	2.0	64
38	Hot-spot analysis for drug discovery targeting protein-protein interactions. <i>Expert Opinion on Drug Discovery</i> , 2018, 13, 327-338.	2.5	64
39	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.	6.6	63
40	pyDockSAXS: protein-protein complex structure by SAXS and computational docking. <i>Nucleic Acids Research</i> , 2015, 43, W356-W361.	6.5	61
41	CCharPPI web server: computational characterization of protein-protein interactions from structure. <i>Bioinformatics</i> , 2015, 31, 123-125.	1.8	61
42	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.	2.0	58
43	Allosteric Conversation in the Androgen Receptor Ligand-Binding Domain Surfaces. <i>Molecular Endocrinology</i> , 2012, 26, 1078-1090.	3.7	58
44	Established and Emerging Trends in Computational Drug Discovery in the Structural Genomics Era. <i>Chemistry and Biology</i> , 2012, 19, 29-41.	6.2	57
45	L amino acid transporter structure and molecular bases for the asymmetry of substrate interaction. <i>Nature Communications</i> , 2019, 10, 1807.	5.8	57
46	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.	2.3	53
47	Identifying interaction motifs in CK2 β - a ubiquitous kinase regulatory subunit. <i>Trends in Biochemical Sciences</i> , 2006, 31, 654-661.	3.7	51
48	Prediction of protein binding sites and hot spots. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 680-698.	6.2	50
49	Blind prediction of interfacial water positions in CAPRI. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 620-632.	1.5	50
50	Brief encounters bolster contacts. <i>Nature</i> , 2006, 444, 279-280.	13.7	46
51	LRR Conservation Mapping to Predict Functional Sites within Protein Leucine-Rich Repeat Domains. <i>PLoS ONE</i> , 2011, 6, e21614.	1.1	46
52	Prediction of protein-binding areas by small-world residue networks and application to docking. <i>BMC Bioinformatics</i> , 2011, 12, 378.	1.2	46
53	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.	1.5	46
54	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.	3.3	46

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55	Improving CAPRI predictions: Optimized desolvation for rigid-body docking. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 60, 308-313.	1.5	45
56	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.	1.5	45
57	Protein-protein Docking and Hot-spot Prediction for Drug Discovery. <i>Current Pharmaceutical Design</i> , 2012, 18, 4607-4618.	0.9	41
58	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.	2.3	41
59	Prediction and scoring of docking poses with pyDock. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 69, 852-858.	1.5	40
60	IRaPPA: information retrieval based integration of biophysical models for protein assembly selection. <i>Bioinformatics</i> , 2017, 33, 1806-1813.	1.8	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. <i>Journal of Biological Chemistry</i> , 2004, 279, 47184-47191.	1.6	30
63	EMMPRIN/CD147 is a novel coreceptor of VEGFR-2 mediating its activation by VEGF. <i>Oncotarget</i> , 2015, 6, 9766-9780.	0.8	30
64	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.	1.5	29
65	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.	2.9	28
66	Structural Basis for Rab1 De-AMPylation by the Legionella pneumophila Effector SidD. <i>PLoS Pathogens</i> , 2013, 9, e1003382.	2.1	28
67	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.	1.5	26
68	Structural assembly of two-domain proteins by rigid-body docking. <i>BMC Bioinformatics</i> , 2008, 9, 441.	1.2	26
69	Structural characterization of unphosphorylated STAT5a oligomerization equilibrium in solution by small angle X-ray scattering. <i>Protein Science</i> , 2009, 18, 716-726.	3.1	26
70	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.	1.5	25
71	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.	6.5	23
72	Intrinsically active MEK variants are differentially regulated by proteinases and phosphatases. <i>Scientific Reports</i> , 2018, 8, 11830.	1.6	22

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73	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.	1.5	20
74	Tetramerization defects of p53 result in aberrant ubiquitylation and transcriptional activity. <i>Molecular Oncology</i> , 2014, 8, 1026-1042.	2.1	20
75	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.	1.5	19
76	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.	1.5	19
77	Docking approaches for modeling multi-molecular assemblies. <i>Current Opinion in Structural Biology</i> , 2020, 64, 59-65.	2.6	18
78	Apoflavodoxin: Structure, stability, and FMN binding. <i>Biochimie</i> , 1998, 80, 813-820.	1.3	17
79	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.	1.5	17
80	Structural and Computational Characterization of Disease-Related Mutations Involved in Protein-Protein Interfaces. <i>International Journal of Molecular Sciences</i> , 2019, 20, 1583.	1.8	17
81	Docking-based identification of small-molecule binding sites at protein-protein interfaces. <i>Computational and Structural Biotechnology Journal</i> , 2020, 18, 3750-3761.	1.9	17
82	pyDockCG: New Coarse-Grained Potential for Protein-Protein Docking. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6032-6039.	1.2	16
83	Structural and energy determinants in protein-RNA docking. <i>Methods</i> , 2017, 118-119, 163-170.	1.9	15
84	pyDockEneRes: per-residue decomposition of protein-protein docking energy. <i>Bioinformatics</i> , 2020, 36, 2284-2285.	1.8	15
85	The "Relevant"™ Stability of Proteins with Equilibrium Intermediates. <i>Scientific World Journal</i> , The, 2002, 2, 1209-1215.	0.8	14
86	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
87	Cell-Dock: high-performance protein-protein docking. <i>Bioinformatics</i> , 2012, 28, 2394-2396.	1.8	14
88	Intrahelical side chain interactions in α -helices: poor correlation between energetics and frequency. <i>FEBS Letters</i> , 1998, 429, 99-103.	1.3	13
89	Docking and scoring: applications to drug discovery in the interactomics era. <i>Expert Opinion on Drug Discovery</i> , 2009, 4, 673-686.	2.5	13
90	Efficient Relaxation of Protein-Protein Interfaces by Discrete Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1222-1229.	2.3	13

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91	Inferring the microscopic surface energy of protein-protein interfaces from mutation data. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 640-650.	1.5	13
92	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.	1.0	13
93	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.	1.8	12
94	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.	1.5	12
95	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.	1.2	11
96	Conformational transitions in human translin enable nucleic acid binding. <i>Nucleic Acids Research</i> , 2013, 41, 9956-9966.	6.5	11
97	Conformational Heterogeneity of Unbound Proteins Enhances Recognition in Protein-Protein Encounters. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3236-3249.	2.3	11
98	Structural and functional characterization of binding sites in metalloproteases based on Optimal Docking Area analysis. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 68, 131-144.	1.5	10
99	In silico docking of urokinase plasminogen activator and integrins. <i>BMC Bioinformatics</i> , 2008, 9, S8.	1.2	10
100	Optimization of protein-protein docking for predicting Fc-protein interactions. <i>Journal of Molecular Recognition</i> , 2016, 29, 555-568.	1.1	10
101	Structural basis for the dominant or recessive character of GLIALCAM mutations found in leukodystrophies. <i>Human Molecular Genetics</i> , 2020, 29, 1107-1120.	1.4	10
102	Docking-based modeling of protein-protein interfaces for extensive structural and functional characterization of missense mutations. <i>PLoS ONE</i> , 2017, 12, e0183643.	1.1	9
103	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.	1.6	9
104	Comment on "protein-protein binding affinity prediction from amino acid sequence". <i>Bioinformatics</i> , 2015, 31, 614-615.	1.8	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. <i>Journal of Clinical Medicine</i> , 2020, 9, 1825.	1.0	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. <i>Plant and Cell Physiology</i> , 2021, 62, 1082-1093.	1.5	7
107	Structural Characterization of Protein-Protein Interactions with pyDockSAXS. <i>Methods in Molecular Biology</i> , 2020, 2112, 131-144.	0.4	7
108	Investigation of the diaphorase reaction of ferredoxin-NADP+ reductase by electrochemical methods. <i>Bioelectrochemistry</i> , 1998, 47, 179-183.	1.0	6

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109	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.	2.3	6
110	Integrative modeling of protein-protein interactions with pyDock for the new docking challenges. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020, 88, 999-1008.	1.5	6
111	Substrate specificity of human metallocarboxypeptidase D: Comparison of the two active carboxypeptidase domains. <i>PLoS ONE</i> , 2017, 12, e0187778.	1.1	6
112	Dissection and prediction of RNA-binding sites on proteins. <i>Biomolecular Concepts</i> , 2010, 1, 345-355.	1.0	5
113	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.	0.5	5
114	UEP: an open-source and fast classifier for predicting the impact of mutations in protein-protein complexes. <i>Bioinformatics</i> , 2021, 37, 334-341.	1.8	5
115	Modeling of Protein Complexes and Molecular Assemblies with pyDock. <i>Methods in Molecular Biology</i> , 2020, 2165, 175-198.	0.4	5
116	Novel treatment strategy for NRAS-mutated melanoma through a selective inhibitor of CD147/VEGFR-2 interaction. <i>Oncogene</i> , 2022, 41, 2254-2264.	2.6	5
117	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.	1.0	4
118	Validated Conformational Ensembles Are Key for the Successful Prediction of Protein Complexes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1830-1837.	2.3	4
119	Modeling Binding Affinity of Pathological Mutations for Computational Protein Design. <i>Methods in Molecular Biology</i> , 2017, 1529, 139-159.	0.4	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. <i>Advances and Applications in Bioinformatics and Chemistry</i> , 2009, , 101.	1.6	3
122	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
123	Unraveling the molecular details of the innate immune response. <i>EBioMedicine</i> , 2016, 9, 7-8.	2.7	1
124	PirePred. <i>Journal of Molecular Diagnostics</i> , 2022, 24, 406-425.	1.2	1
125	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
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.	2.6	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.	2.6	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.	2.6	0
132	Drug Design on the Cell BE. Chapman & Hall/CRC Computational Science, 2010, , 331-350.	0.5	0