Community-Wide Assessment of Protein-Interface Mod
Design Methodology

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Citation Report

#	Article	IF	Citations
1	Proteinâ€“protein binding affinity prediction on a diverse set of structures. Bioinformatics, 2011, 27, 3002-3009.	1.8	103
2	Protein-protein Docking and Hot-spot Prediction for Drug Discovery. Current Pharmaceutical Design, 2012, 18, 4607-4618.	0.9	41
3	Engineered Oligomerization State of OmpF Protein through Computational Design Decouples Oligomer Dissociation from Unfolding. Journal of Molecular Biology, 2012, 419, 89-101.	2.0	28
4	Role of the Biomolecular Energy Gap in Protein Design, Structure, and Evolution. Cell, 2012, 149, 262-273.	13.5	94
5	Combining different design strategies for rational affinity maturation of the MICAâ€NKG2D interface. Protein Science, 2012, 21, 1396-1402.	3.1	4
6	Prediction of proteinâ€“protein binding free energies. Protein Science, 2012, 21, 396-404.	3.1	74
7	Scoring protein interaction decoys using exposed residues (SPIDER): A novel multibody interaction scoring function based on frequent geometric patterns of interfacial residues. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2207-2217.	1.5	41
8	Multiscale modeling of macromolecular biosystems. Briefings in Bioinformatics, 2012, 13, 395-405.	3.2	29
9	Computational Design of Self-Assembling Protein Nanomaterials with Atomic Level Accuracy. Science, 2012, 336, 1171-1174.	6.0	588
10	Dissecting genomic regulatory elements in vivo. Nature Biotechnology, 2012, 30, 504-506.	9.4	9
11	Next-generation protein engineering targets influenza. Nature Biotechnology, 2012, 30, 502-504.	9.4	1
12	Defining the limits of homology modeling in informationâ€driven protein docking. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2119-2128.	1.5	63
13	Dataâ€driven models for protein interaction and design. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2221-2228.	1.5	5
14	Computational design of proteinâ€“protein interactions. Current Opinion in Structural Biology, 2013, 23, 903-910.	2.6	53
15	The targets of CAPRI rounds 20â€“27. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2075-2081.	1.5	14
16	New molecular interaction of IIA^{Ntr} and HPr from Burkholderia pseudomallei identified by Xâ€ray crystallography and docking studies. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1499-1508.	1.5	2
17	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
18	Molecular origins of binding affinity: seeking the Archimedean point. Current Opinion in Structural Biology, 2013, 23, 868-877.	2.6	37

#	Article	IF	Citations
19	Scoring functions for proteinâ€“protein interactions. Current Opinion in Structural Biology, 2013, 23, 862-867.	2.6	87
20	Docking Predictions of Protein-Protein Interactions and Their Assessment: The CAPRI Experiment. Focus on Structural Biology, 2013, , 87-104.	0.1	5
21	Computational Design of a Protein-Based Enzyme Inhibitor. Journal of Molecular Biology, 2013, 425, 3563-3575.	2.0	85
22	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
23	Emerging themes in the computational design of novel enzymes and proteinâ€“protein interfaces. FEBS Letters, 2013, 587, 1147-1154.	1.3	46
24	Strategies to control the binding mode of de novo designed protein interactions. Current Opinion in Structural Biology, 2013, 23, 639-646.	2.6	19
25	Docking, scoring, and affinity prediction in CAPRI. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2082-2095.	1.5	216
26	The scoring of poses in protein-protein docking: current capabilities and future directions. BMC Bioinformatics, 2013, 14, 286.	1.2	98
28	Uncovering the Determinants of a Highly Perturbed Tyrosine pKa in the Active Site of Ketosteroid Isomerase. Biochemistry, 2013, 52, 7840-7855.	1.2	37
29	Redesign of a cross-reactive antibody to dengue virus with broad-spectrum activity and increased in vivo potency. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E1555-64.	3.3	58
30	A comparison of successful and failed protein interface designs highlights the challenges of designing buried hydrogen bonds. Protein Science, 2013, 22, 74-82.	3.1	166
31	Energy Functions in De Novo Protein Design: Current Challenges and Future Prospects. Annual Review of Biophysics, 2013, 42, 315-335.	4.5	75
32	Computational Design of Novel Protein Binders and Experimental Affinity Maturation. Methods in Enzymology, 2013, 523, 1-19.	0.4	38
33	Energetics of oligomeric protein folding and association. Archives of Biochemistry and Biophysics, 2013, 531, 44-64.	1.4	47
34	On the binding affinity of macromolecular interactions: daring to ask why proteins interact. Journal of the Royal Society Interface, 2013, 10, 20120835.	1.5	353
35	Increasing Affinity of Interferon-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="M1"><mml:mrow><mml:mi mathvariant="bold">Î³</mml:mi></mml:mrow></mml:math>Receptor 1 to Interferon-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="M2"><mml:mrow><mml:mi mathvariant="bold">Î³</mml:mi></mml:mrow></mml:math>by Computer-Aided Design. BioMed Research International, 2013, 2013, 1-12.	0.9	12
36	Using physical potentials and learned models to distinguish native binding interfaces from de novo designed interfaces that do not bind. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1919-1930.	1.5	5
37	Extending RosettaDock with water, sugar, and pH for prediction of complex structures and affinities for CAPRI rounds 20â€“27. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2201-2209.	1.5	22

#	Article	IF	Citations
38	Using the concept of transient complex for affinity predictions in CAPRI rounds 20â€“27 and beyond. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2229-2236.	1.5	7
39	Performance of ZDOCK in CAPRI rounds 20â€“26. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2175-2182.	1.5	22
40	Exploring Angular Distance in Protein-Protein Docking Algorithms. PLoS ONE, 2013, 8, e56645.	1.1	11
41	Parallel In Vivo DNA Assembly by Recombination: Experimental Demonstration and Theoretical Approaches. PLoS ONE, 2013, 8, e56854.	1.1	7
42	Protein-RNA Complexes and Efficient Automatic Docking: Expanding RosettaDock Possibilities. PLoS ONE, 2014, 9, e108928.	1.1	30
43	Protein-Protein Interface Detection Using the Energy Centrality Relationship (ECR) Characteristic of Proteins. PLoS ONE, 2014, 9, e97115.	1.1	2
44	Physicsâ€based enzyme design: Predicting binding affinity and catalytic activity. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3397-3409.	1.5	39
45	Score_set: A CAPRI benchmark for scoring protein complexes. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3163-3169.	1.5	72
46	Proteins Feel More Than They See: Fine-Tuning of Binding Affinity by Properties of the Non-Interacting Surface. Journal of Molecular Biology, 2014, 426, 2632-2652.	2.0	103
47	Mapping of the Binding Landscape for a Picomolar Protein-Protein Complex through Computation and Experiment. Structure, 2014, 22, 636-645.	1.6	18
48	Signatures of nâ†'Ï€* interactions in proteins. Protein Science, 2014, 23, 284-288.	3.1	82
49	An improved Protein G with higher affinity for human/rabbit IgG Fc domains exploiting a computationally designed polar network. Protein Engineering, Design and Selection, 2014, 27, 127-134.	1.0	21
50	Protein engineering and the use of molecular modeling and simulation: The case of heterodimeric Fc engineering. Methods, 2014, 65, 77-94.	1.9	13
51	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	1.5	50
52	Novel RANK Antagonists for the Treatment of Bone-Resorptive Disease: Theoretical Predictions and Experimental Validation. Journal of Bone and Mineral Research, 2014, 29, 1466-1477.	3.1	12
53	Scoring docking conformations using predicted protein interfaces. BMC Bioinformatics, 2014, 15, 171.	1.2	14
54	Evolution of protein interactions: From interactomes to interfaces. Archives of Biochemistry and Biophysics, 2014, 554, 65-75.	1.4	49
55	Forces stabilizing proteins. FEBS Letters, 2014, 588, 2177-2184.	1.3	273

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56	An accurate binding interaction model in de novo computational protein design of interactions: If you build it, they will bind. Journal of Structural Biology, 2014, 185, 136-146.	1.3	12
58	Inferring the microscopic surface energy of proteinâ€“protein interfaces from mutation data. Proteins: Structure, Function and Bioinformatics, 2015, 83, 640-650.	1.5	13
59	Non-interacting surface solvation and dynamics in protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2015, 83, 445-458.	1.5	22
60	Linking structural features of protein complexes and biological function. Protein Science, 2015, 24, 1486-1494.	3.1	33
61	AbDesign: An algorithm for combinatorial backbone design guided by natural conformations and sequences. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1385-1406.	1.5	86
62	Surfing the Protein-Protein Interaction Surface Using Docking Methods: Application to the Design of PPI Inhibitors. Molecules, 2015, 20, 11569-11603.	1.7	61
63	Contacts-based prediction of binding affinity in proteinâ€“protein complexes. ELife, 2015, 4, e07454.	2.8	385
64	Protein design: Past, present, and future. Biopolymers, 2015, 104, 334-350.	1.2	38
65	Computational design and experimental verification of a symmetric protein homodimer. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 10714-10719.	3.3	34
66	Adaptability of protein structures to enable functional interactions and evolutionary implications. Current Opinion in Structural Biology, 2015, 35, 17-23.	2.6	104
67	Using Molecular Dynamics Simulations as an Aid in the Prediction of Domain Swapping of Computationally Designed Protein Variants. Journal of Molecular Biology, 2015, 427, 2697-2706.	2.0	11
68	CCharPPI web server: computational characterization of proteinâ€“protein interactions from structure. Bioinformatics, 2015, 31, 123-125.	1.8	61
69	Structural Interface Forms and Their Involvement in Stabilization of Multidomain Proteins or Protein Complexes. International Journal of Molecular Sciences, 2016, 17, 1741.	1.8	29
70	Molecular docking as a popular tool in drug design, an in silico travel. Advances and Applications in Bioinformatics and Chemistry, 2016, Volume 9, 1-11.	1.6	182
71	s<scp>DFIRE</scp>: Sequenceâ€specific statistical energy function for protein structure prediction by decoy selections. Journal of Computational Chemistry, 2016, 37, 1119-1124.	1.5	16
72	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
73	ProtLID, a Residue-Based Pharmacophore Approach to Identify Cognate Protein Ligands in the Immunoglobulin Superfamily. Structure, 2016, 24, 2217-2226.	1.6	10
74	Motif-Driven Design of Proteinâ€“Protein Interfaces. Methods in Molecular Biology, 2016, 1414, 285-304.	0.4	34

#	Article	IF	Citations
75	Deep Mutational Scans as a Guide to Engineering High Affinity T Cell Receptor Interactions with Peptide-bound Major Histocompatibility Complex. Journal of Biological Chemistry, 2016, 291, 24566-24578.	1.6	42
76	A generalized framework for computational design and mutational scanning of T-cell receptor binding interfaces. Protein Engineering, Design and Selection, 2016, 29, 595-606.	1.0	16
77	Model Building of Antibodyâ€“Antigen Complex Structures Using GBSA Scores. Journal of Chemical Information and Modeling, 2016, 56, 2005-2012.	2.5	16
78	Accurate design of megadalton-scale two-component icosahedral protein complexes. Science, 2016, 353, 389-394.	6.0	466
79	<scp>AB</scp> â€Bind: Antibody binding mutational database for computational affinity predictions. Protein Science, 2016, 25, 393-409.	3.1	110
80	Crystal Structure of Streptococcus pyogenes Cas1 and Its Interaction with Csn2 in the Type II CRISPR-Cas System. Structure, 2016, 24, 70-79.	1.6	21
81	Design and fine-tuning redox potentials of metalloproteins involved in electron transfer in bioenergetics. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 557-581.	0.5	130
82	Trade-offs between enzyme fitness and solubility illuminated by deep mutational scanning. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2265-2270.	3.3	114
83	Prediction of Biomolecular Complexes. , 2017, , 265-292.		11
85	Drug Target miRNA. Methods in Molecular Biology, 2017, , .	0.4	2
86	FlexPepDock lessons from CAPRI peptideâ€“protein rounds and suggested new criteria for assessment of model quality and utility. Proteins: Structure, Function and Bioinformatics, 2017, 85, 445-462.	1.5	19
87	BindML/BindML+: Detecting Protein-Protein Interaction Interface Propensity from Amino Acid Substitution Patterns. Methods in Molecular Biology, 2017, 1529, 279-289.	0.4	4
88	Elucidating Mechanisms of Molecular Recognition Between Human Argonaute and miRNA Using Computational Approaches. Methods in Molecular Biology, 2017, 1517, 251-275.	0.4	1
89	The computational prediction of protein assemblies. Current Opinion in Structural Biology, 2017, 46, 170-175.	2.6	4
90	Protein social behavior makes a stronger signal for partner identification than surface geometry. Proteins: Structure, Function and Bioinformatics, 2017, 85, 137-154.	1.5	18
91	Modeling proteinâ€“protein and proteinâ€“peptide complexes: CAPRI 6th edition. Proteins: Structure, Function and Bioinformatics, 2017, 85, 359-377.	1.5	198
92	Structure-based cross-docking analysis of antibodyâ€“antigen interactions. Scientific Reports, 2017, 7, 8145.	1.6	37
93	Comparing side chain packing in soluble proteins, proteinâ€protein interfaces, and transmembrane proteins. Proteins: Structure, Function and Bioinformatics, 2018, 86, 581-591.	1.5	8

#	Article	IF	Citations
94	The challenge of modeling protein assemblies: the CASP12â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2018, 86, 257-273.	1.5	85
95	Ultrahigh specificity in a network of computationally designed protein-interaction pairs. Nature Communications, 2018, 9, 5286.	5.8	49
96	Third generation antibody discovery methods:in silicorational design. Chemical Society Reviews, 2018, 47, 9137-9157.	18.7	94
97	Antibody Affinity Maturation by Computational Design. Methods in Molecular Biology, 2018, 1827, 15-34.	0.4	19
98	Local Interaction Signal Analysis Predicts Protein-Protein Binding Affinity. Structure, 2018, 26, 905-915.e4.	1.6	24
99	Blind prediction of homoâ€and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	1.5	99
100	Void distributions reveal structural link between jammed packings and protein cores. Physical Review E, 2019, 99, 022416.	0.8	9
101	Unveiling the nâ†'Ï€* interactions in dipeptides. Communications Chemistry, 2019, 2, .	2.0	30
102	Structure-Based Drug Design with a Special Emphasis on Herbal Extracts. Challenges and Advances in Computational Chemistry and Physics, 2019, , 271-305.	0.6	0
103	Modeling proteinâ€protein, proteinâ€peptide, and proteinâ€oligosaccharide complexes: CAPRI 7th edition. Proteins: Structure, Function and Bioinformatics, 2020, 88, 916-938.	1.5	96
104	Engineered receptors for human cytomegalovirus that are orthogonal to normal human biology. PLoS Pathogens, 2020, 16, e1008647.	2.1	11
105	Prediction of peptide binding to MHC using machine learning with sequence and structure-based feature sets. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129535.	1.1	15
106	The Electrostatic Features of Dengue Virus Capsid Assembly. Journal of Computational Biophysics and Chemistry, 2021, 20, 201-207.	1.0	7
107	Residue-based pharmacophore approaches to study proteinâ€“protein interactions. Current Opinion in Structural Biology, 2021, 67, 205-211.	2.6	4
108	Community-Wide Experimental Evaluation of the PROSS Stability-Design Method. Journal of Molecular Biology, 2021, 433, 166964.	2.0	42
109	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
110	Improvement of the Proteinâ€“Protein Docking Prediction by Introducing a Simple Hydrophobic Interaction Model: An Application to Interaction Pathway Analysis. Lecture Notes in Computer Science, 2012, , 178-187.	1.0	10
111	Prediction of Protein-Protein Binding Interfaces. Focus on Structural Biology, 2013, , 105-133.	0.1	4

#	Article	IF	Citations
112	Generating quantitative binding landscapes through fractional binding selections combined with deep sequencing and data normalization. Nature Communications, 2020, 11, 297.	5.8	10
113	Markov State Models Reveal a Two-Step Mechanism of miRNA Loading into the Human Argonaute Protein: Selective Binding followed by Structural Re-arrangement. PLoS Computational Biology, 2015, 11, e1004404.	1.5	56
114	Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics. PLoS Computational Biology, 2016, 12, e1004619.	1.5	188
115	ATTRACT-EM: A New Method for the Computational Assembly of Large Molecular Machines Using Cryo-EM Maps. PLoS ONE, 2012, 7, e49733.	1.1	45
116	How Structure Defines Affinity in Protein-Protein Interactions. PLoS ONE, 2014, 9, e110085.	1.1	77
117	Protein-Protein Interactions and Prediction: A Comprehensive Overview. Protein and Peptide Letters, 2013, 21, 779-789.	0.4	19
119	Using diverse potentials and scoring functions for the development of improved machine-learned models for proteinâ€“ligand affinity and docking pose prediction. Journal of Computer-Aided Molecular Design, 2021, 35, 1095-1123.	1.3	3
120	Proteinâ€“Protein Docking: Past, Present, and Future. Protein Journal, 2022, 41, 1-26.	0.7	12
122	Polydopamine nanospheres coated with bovine serum albumin permit enhanced cell differentiation: fundamental mechanism and practical application for protein coating formation. Nanoscale, 2021, 13, 20098-20110.	2.8	14
123	Tertiary motifs as building blocks for the design of proteinâ€binding peptides. Protein Science, 2022, 31, .	3.1	8
124	Spatial organization of hydrophobic and charged residues affects protein thermal stability and binding affinity. Scientific Reports, 2022, 12, .	1.6	21
125	Assessing and enhancing foldability in designed proteins. Protein Science, 2022, 31, .	3.1	10
126	Proteinâ€“protein interaction prediction methods: from docking-based to AI-based approaches. Biophysical Reviews, 2022, 14, 1341-1348.	1.5	5
127	Critical Assessment of Methods for Predicting the 3D Structure of Proteins and Protein Complexes. Annual Review of Biophysics, 2023, 52, 183-206.	4.5	16
128	Artificial Neural Network to Predict Structure-based Protein-protein Free Energy of Binding from Rosetta calculated Properties. Physical Chemistry Chemical Physics, 0, , .	1.3	0