

Ram Samudrala

List of Publications by Year in descending order

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94
papers

5,264
citations

136950
32
h-index

95266
68
g-index

177
all docs

177
docs citations

177
times ranked

6324
citing authors

#	ARTICLE	IF	CITATIONS
1	The Genomes of <i>Oryza sativa</i> : A History of Duplications. <i>PLoS Biology</i> , 2005, 3, e38.	5.6	808
2	Data access for the 1,000 Plants (1KP) project. <i>GigaScience</i> , 2014, 3, 17.	6.4	582
3	An all-atom distance-dependent conditional probability discriminatory function for protein structure prediction 1 Edited by F. Cohen. <i>Journal of Molecular Biology</i> , 1998, 275, 895-916.	4.2	429
4	Decoys â€” Us: A database of incorrect conformations to improve protein structure prediction. <i>Protein Science</i> , 2000, 9, 1399-1401.	7.6	215
5	Accurate Prediction of Secreted Substrates and Identification of a Conserved Putative Secretion Signal for Type III Secretion Systems. <i>PLoS Pathogens</i> , 2009, 5, e1000375.	4.7	177
6	Ab initio construction of protein tertiary structures using a hierarchical approach. <i>Journal of Molecular Biology</i> , 2000, 300, 171-185.	4.2	162
7	A graph-theoretic algorithm for comparative modeling of protein structure. <i>Journal of Molecular Biology</i> , 1998, 279, 287-302.	4.2	133
8	Neutral evolution of â€”non-codingâ€” complementary DNAs. <i>Nature</i> , 2004, 431, 1-2.	27.8	127
9	Novel paradigms for drug discovery: computational multitarget screening. <i>Trends in Pharmacological Sciences</i> , 2008, 29, 62-71.	8.7	127
10	Computational Prediction of Type III and IV Secreted Effectors in Gram-Negative Bacteria. <i>Infection and Immunity</i> , 2011, 79, 23-32.	2.2	113
11	Structural polymorphism and diversifying selection on the pregnancy malaria vaccine candidate VAR2CSA. <i>Molecular and Biochemical Parasitology</i> , 2007, 155, 103-112.	1.1	111
12	Structural Optimization and De Novo Design of Dengue Virus Entry Inhibitory Peptides. <i>PLoS Neglected Tropical Diseases</i> , 2010, 4, e721.	3.0	99
13	Ab Initio fold prediction of small helical proteins using distance geometry and knowledge-based scoring functions 1 Edited by F. Cohen. <i>Journal of Molecular Biology</i> , 1999, 290, 267-281.	4.2	89
14	Caries induced cytokine network in the odontoblast layer of human teeth. <i>BMC Immunology</i> , 2011, 12, 9.	2.2	88
15	Improvement in protein functional site prediction by distinguishing structural and functional constraints on protein family evolution using computational design. <i>Nucleic Acids Research</i> , 2005, 33, 5861-5867.	14.5	78
16	CANDO and the infinite drug discovery frontier. <i>Drug Discovery Today</i> , 2014, 19, 1353-1363.	6.4	67
17	Ab initio protein structure prediction using a combined hierarchical approach. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 37, 194-198.	2.6	66
18	Identifying inhibitors of the SARS coronavirus proteinase. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2003, 13, 3989-3992.	2.2	63

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19	Improved prediction of HIV-1 protease-inhibitor binding energies by molecular dynamics simulations. BMC Structural Biology, 2003, 3, 2.	2.3	62
20	PROTINFO: new algorithms for enhanced protein structure predictions. Nucleic Acids Research, 2005, 33, W77-W80.	14.5	60
21	Improved protein structure selection using decoy-dependent discriminatory functions. BMC Structural Biology, 2004, 4, 8.	2.3	56
22	Functional annotation from predicted protein interaction networks. Bioinformatics, 2005, 21, 3217-3226.	4.1	54
23	Protein mimetic amyloid inhibitor potently abrogates cancer-associated mutant p53 aggregation and restores tumor suppressor function. Nature Communications, 2021, 12, 3962.	12.8	53
24	Exploring Polypharmacology in Drug Discovery and Repurposing Using the CANDO Platform. Current Pharmaceutical Design, 2016, 22, 3109-3123.	1.9	50
25	A comprehensive analysis of 40 blind protein structure predictions. , 2002, 2, 3.		47
26	Viral entry inhibitors block dengue antibody-dependent enhancement in vitro. Antiviral Research, 2011, 89, 71-74.	4.1	47
27	Combating Ebola with Repurposed Therapeutics Using the CANDO Platform. Molecules, 2016, 21, 1537.	3.8	46
28	Simple Linear Model Provides Highly Accurate Genotypic Predictions of HIV-1 Drug Resistance. Antiviral Therapy, 2004, 9, 343-352.	1.0	45
29	Accurate and automated classification of protein secondary structure with PsiCSI. Protein Science, 2003, 12, 288-295.	7.6	44
30	Prediction of HIV-1 Protease Inhibitor Resistance using a Proteinâ€“Inhibitor Flexible Docking Approach. Antiviral Therapy, 2005, 10, 157-166.	1.0	40
31	PROTINFO: secondary and tertiary protein structure prediction. Nucleic Acids Research, 2003, 31, 3296-3299.	14.5	38
32	Protein Meta-Functional Signatures from Combining Sequence, Structure, Evolution, and Amino Acid Property Information. PLoS Computational Biology, 2008, 4, e1000181.	3.2	37
33	Constructing side chains on near-native main chains for ab initio protein structure prediction. Protein Engineering, Design and Selection, 2000, 13, 453-457.	2.1	36
34	CANDOCK: Chemical Atomic Network-Based Hierarchical Flexible Docking Algorithm Using Generalized Statistical Potentials. Journal of Chemical Information and Modeling, 2020, 60, 1509-1527.	5.4	36
35	Disguising itselfâ€“insights into Plasmodium falciparum binding and immune evasion from the DBL crystal structure. Molecular and Biochemical Parasitology, 2006, 148, 1-9.	1.1	34
36	A COMBINED APPROACH FOR AB INITIO CONSTRUCTION OF LOW RESOLUTION PROTEIN TERTIARY STRUCTURES FROM SEQUENCE. , 1998, , 505-16.		34

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37	Multiscale Modelling of Relationships between Protein Classes and Drug Behavior Across all Diseases Using the CANDO Platform. Mini-Reviews in Medicinal Chemistry, 2015, 15, 705-717.	2.4	34
38	Identification of Potential Multitarget Antimalarial Drugs. JAMA - Journal of the American Medical Association, 2005, 294, 1487.	7.4	28
39	A Systematic Review of Computational Drug Discovery, Development, and Repurposing for Ebola Virus Disease Treatment. Molecules, 2017, 22, 1777.	3.8	28
40	Ab initio protein structure prediction using a combined hierarchical approach. Proteins: Structure, Function and Bioinformatics, 1999, 37, 194-198.	2.6	27
41	Distance geometry generates native-like folds for small helical proteins using the consensus distances of predicted protein structures. Protein Science, 1998, 7, 1998-2003.	7.6	26
42	A generalized knowledge-based discriminatory function for biomolecular interactions. Proteins: Structure, Function and Bioinformatics, 2009, 76, 115-128.	2.6	26
43	Confronting the problem of interconnected structural changes in the comparative modeling of proteins. Proteins: Structure, Function and Bioinformatics, 1995, 23, 327-336.	2.6	25
44	FSSA: a novel method for identifying functional signatures from structural alignments. Bioinformatics, 2005, 21, 2969-2977.	4.1	25
45	Crystal Structure and Mutational Analysis of the DaaE Adhesin of Escherichia coli. Journal of Biological Chemistry, 2006, 281, 22367-22377.	3.4	24
46	Fingerprinting CANDO: Increased Accuracy with Structure- and Ligand-Based Shotgun Drug Repurposing. ACS Omega, 2019, 4, 17393-17403.	3.5	24
47	Identifying Protein Features Responsible for Improved Drug Repurposing Accuracies Using the CANDO Platform: Implications for Drug Design. Molecules, 2019, 24, 167.	3.8	24
48	A synthetic small molecule stalls pre-mRNA splicing by promoting an early-stage U2AF2-RNA complex. Cell Chemical Biology, 2021, 28, 1145-1157.e6.	5.2	24
49	The Enzymatic and Metabolic Capabilities of Early Life. PLoS ONE, 2012, 7, e39912.	2.5	24
50	Prediction of HIV-1 protease inhibitor resistance using a protein-inhibitor flexible docking approach. Antiviral Therapy, 2005, 10, 157-66.	1.0	24
51	Shotgun drug repurposing biotechnology to tackle epidemics and pandemics. Drug Discovery Today, 2020, 25, 1126-1128.	6.4	22
52	Simple linear model provides highly accurate genotypic predictions of HIV-1 drug resistance. Antiviral Therapy, 2004, 9, 343-52.	1.0	22
53	PIRSpred: a web server for reliable HIV-1 protein-inhibitor resistance/susceptibility prediction. Trends in Microbiology, 2005, 13, 150-151.	7.7	21
54	Protinfo PPC: A web server for atomic level prediction of protein complexes. Nucleic Acids Research, 2009, 37, W519-W525.	14.5	21

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55	cando.py: Open Source Software for Predictive Bioanalytics of Large Scale Drug-Protein-Disease Data. Journal of Chemical Information and Modeling, 2020, 60, 4131-4136.	5.4	21
56	Enhanced functional information from predicted protein networks. Trends in Biotechnology, 2004, 22, 60-62.	9.3	18
57	BIOVERSE: enhancements to the framework for structural, functional and contextual modeling of proteins and proteomes. Nucleic Acids Research, 2005, 33, W324-W325.	14.5	18
58	Identification of potential HIV-1 targets of minocycline. Bioinformatics, 2007, 23, 2797-2799.	4.1	18
59	Computational chemoproteomics to understand the role of selected psychoactives in treating mental health indications. Scientific Reports, 2019, 9, 13155.	3.3	18
60	Exploration of interaction scoring criteria in the CANDO platform. BMC Research Notes, 2019, 12, 318.	1.4	18
61	Evaluating the performance of drug-repurposing technologies. Drug Discovery Today, 2022, 27, 49-64.	6.4	18
62	fast_protein_cluster: parallel and optimized clustering of large-scale protein modeling data. Bioinformatics, 2014, 30, 1774-1776.	4.1	16
63	Heptad-Repeat-2 Mutations Enhance the Stability of the Enfuvirtide-Resistant HIV-1 gp41 Hairpin Structure. Antiviral Therapy, 2005, 10, 893-900.	1.0	16
64	Handling context-sensitivity in protein structures using graph theory: Bona fide prediction. Proteins: Structure, Function and Bioinformatics, 1997, 29, 43-49.	2.6	15
65	Virtual screening of HIV-1 protease inhibitors against human cytomegalovirus protease using docking and molecular dynamics. Aids, 2005, 19, 529-531.	2.2	15
66	Accelerated protein structure comparison using TM-score-GPU. Bioinformatics, 2012, 28, 2191-2192.	4.1	15
67	Antivirogram or Phenosense: A Comparison of their Reproducibility and an Analysis of their Correlation. Antiviral Therapy, 2004, 9, 703-712.	1.0	15
68	Improving the accuracy of template-based predictions by mixing and matching between initial models. BMC Structural Biology, 2008, 8, 24.	2.3	13
69	Improved accuracy of HIV-1 genotypic susceptibility interpretation using a consensus approach. Aids, 2004, 18, 1858-1859.	2.2	12
70	Prediction and Integration of Regulatory and Protein-Protein Interactions. Methods in Molecular Biology, 2009, 541, 101-143.	0.9	12
71	Multiscale Virtual Screening Optimization for Shotgun Drug Repurposing Using the CANDO Platform. Molecules, 2021, 26, 2581.	3.8	12
72	GPU-QJ, a fast method for calculating root mean square deviation (RMSD) after optimal superposition. BMC Research Notes, 2011, 4, 97.	1.4	11

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73	Diversity of protein structures and difficulties in fold recognition: the curious case of protein G. F1000 Biology Reports, 2009, 1, 69.	4.0	11
74	Scoring Functions for ab initio Protein Structure Prediction. , 2000, 143, 223-245.		10
75	Scoring Functions for De Novo Protein Structure Prediction Revisited. , 2008, 413, 243-281.		10
76	Heptad-repeat-2 mutations enhance the stability of the enfuvirtide-resistant HIV-1 gp41 hairpin structure. Antiviral Therapy, 2005, 10, 893-900.	1.0	10
77	HIVâ€™s Genotypic Drugâ€™Resistance Interpretation Algorithms Need to Include Hypersusceptibilityâ€™Associated Mutations. Journal of Infectious Diseases, 2004, 190, 2055-2056.	4.0	8
78	A novel method for predicting and using distance constraints of high accuracy for refining protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2009, 77, 220-234.	2.6	8
79	A fluorescence-based, gain-of-signal, live cell system to evaluate SARS-CoV-2 main protease inhibition. Antiviral Research, 2021, 195, 105183.	4.1	8
80	LoCo: a novel main chain scoring function for protein structure prediction based on local coordinates. BMC Bioinformatics, 2011, 12, 368.	2.6	7
81	Composite Sequenceâ€™Structure Stability Models as Screening Tools for Identifying Vulnerable Targets for HIV Drug and Vaccine Development. Viruses, 2015, 7, 5718-5735.	3.3	7
82	De Novo Protein Structure Prediction. Biological and Medical Physics Series, 2007, , 43-63.	0.4	7
83	A Deep-Learning Proteomic-Scale Approach for Drug Design. Pharmaceuticals, 2021, 14, 1277.	3.8	7
84	Identifying Protein Features and Pathways Responsible for Toxicity Using Machine Learning and Tox21: Implications for Predictive Toxicology. Molecules, 2022, 27, 3021.	3.8	7
85	Structure Prediction of Partial-Length Protein Sequences. International Journal of Molecular Sciences, 2013, 14, 14892-14907.	4.1	6
86	Inferring Molecular Interactions Pathways from eQTL Data. Methods in Molecular Biology, 2009, 541, 211-223.	0.9	5
87	Proteomic Network Analysis of Bronchoalveolar Lavage Fluid in Ex-Smokers to Discover Implicated Protein Targets and Novel Drug Treatments for Chronic Obstructive Pulmonary Disease. Pharmaceuticals, 2022, 15, 566.	3.8	5
88	Protein structure prediction based on optimal hydrophobic core formation. , 2012, , .		3
89	Accurate Prediction of Inhibitor Binding to HIV-1 Protease Using CANDOCK. Frontiers in Chemistry, 2021, 9, 775513.	3.6	3
90	Modeling genome structure and function. Pure and Applied Chemistry, 2002, 74, 907-914.	1.9	2

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91	Rv0100, a proposed acyl carrier protein in <i>Mycobacterium tuberculosis</i> : expression, purification and crystallization. Acta Crystallographica Section F, Structural Biology Communications, 2019, 75, 646-651.	0.8	1
92	The Promise and Challenge of Digital Biology. Journal of Bioengineering & Biomedical Science, 2013, 03, .	0.2	1
93	Probing structure-function relationships of the DNA polymerase alpha-associated zinc-finger protein using computational approaches. , 1999, , 179-90.		1
94	Mycobacterium Cytidylate Kinase Appears to Be an Undruggable Target. Journal of Biomolecular Screening, 2016, 21, 695-700.	2.6	0