Ram Samudrala

List of Publications by Year
in descending order

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	Evaluating the performance of drug-repurposing technologies. Drug Discovery Today, 2022, 27, 49-64.	6.4	18
2	Identifying Protein Features and Pathways Responsible for Toxicity Using Machine Learning and Tox21: Implications for Predictive Toxicology. Molecules, 2022, 27, 3021.	3.8	7
3	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
4	Multiscale Virtual Screening Optimization for Shotgun Drug Repurposing Using the CANDO Platform. Molecules, 2021, 26, 2581.	3.8	12
5	Protein mimetic amyloid inhibitor potently abrogates cancer-associated mutant p53 aggregation and restores tumor suppressor function. Nature Communications, 2021, 12, 3962.	12.8	53
6	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
7	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
8	Accurate Prediction of Inhibitor Binding to HIV-1 Protease Using CANDOCK. Frontiers in Chemistry, 2021, 9, 775513.	3.6	3
9	A Deep-Learning Proteomic-Scale Approach for Drug Design. Pharmaceuticals, 2021, 14, 1277.	3.8	7
10	Shotgun drug repurposing biotechnology to tackle epidemics and pandemics. Drug Discovery Today, 2020, 25, 1126-1128.	6.4	22
11	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
12	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
13	Fingerprinting CANDO: Increased Accuracy with Structure- and Ligand-Based Shotgun Drug Repurposing. ACS Omega, 2019, 4, 17393-17403.	3.5	24
14	Computational chemoproteomics to understand the role of selected psychoactives in treating mental health indications. Scientific Reports, 2019, 9, 13155.	3.3	18
15	Identifying Protein Features Responsible for Improved Drug Repurposing Accuracies Using the CANDO Platform: Implications for Drug Design. Molecules, 2019, 24, 167.	3.8	24
16	Exploration of interaction scoring criteria in the CANDO platform. BMC Research Notes, 2019, 12, 318.	1.4	18
17	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
18	A Systematic Review of Computational Drug Discovery, Development, and Repurposing for Ebola Virus Disease Treatment. Molecules, 2017, 22, 1777.	3.8	28

#	Article	IF	Citations
19	Combating Ebola with Repurposed Therapeutics Using the CANDO Platform. Molecules, 2016, 21, 1537.	3.8	46
20	Mycobacterium Cytidylate Kinase Appears to Be an Undruggable Target. Journal of Biomolecular Screening, 2016, 21, 695-700.	2.6	0
21	Exploring Polypharmacology in Drug Discovery and Repurposing Using the CANDO Platform. Current Pharmaceutical Design, 2016, 22, 3109-3123.	1.9	50
22	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
23	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
24	fast_protein_cluster: parallel and optimized clustering of large-scale protein modeling data. Bioinformatics, 2014, 30, 1774-1776.	4.1	16
25	Data access for the 1,000 Plants (1KP) project. GigaScience, 2014, 3, 17.	6.4	582
26	CANDO and the infinite drug discovery frontier. Drug Discovery Today, 2014, 19, 1353-1363.	6.4	67
27	Structure Prediction of Partial-Length Protein Sequences. International Journal of Molecular Sciences, 2013, 14, 14892-14907.	4.1	6
28	The Promise and Challenge of Digital Biology. Journal of Bioengineering & Biomedical Science, 2013, 03, .	0.2	1
29	Accelerated protein structure comparison using TM-score-GPU. Bioinformatics, 2012, 28, 2191-2192.	4.1	15
30	Protein structure prediction based on optimal hydrophobic core formation. , 2012, , .		3
31	The Enzymatic and Metabolic Capabilities of Early Life. PLoS ONE, 2012, 7, e39912.	2.5	24
32	GPU-Q-J, a fast method for calculating root mean square deviation (RMSD) after optimal superposition. BMC Research Notes, 2011, 4, 97.	1.4	11
33	Viral entry inhibitors block dengue antibody-dependent enhancement in vitro. Antiviral Research, 2011, 89, 71-74.	4.1	47
34	LoCo: a novel main chain scoring function for protein structure prediction based on local coordinates. BMC Bioinformatics, 2011, 12, 368.	2.6	7
35	Caries induced cytokine network in the odontoblast layer of human teeth. BMC Immunology, 2011, 12, 9.	2.2	88
36	Computational Prediction of Type III and IV Secreted Effectors in Gram-Negative Bacteria. Infection and Immunity, 2011, 79, 23-32.	2.2	113

#	Article	IF	Citations
37	Structural Optimization and De Novo Design of Dengue Virus Entry Inhibitory Peptides. PLoS Neglected Tropical Diseases, 2010, 4, e721.	3.0	99
38	Protinfo PPC: A web server for atomic level prediction of protein complexes. Nucleic Acids Research, 2009, 37, W519-W525.	14.5	21
39	Accurate Prediction of Secreted Substrates and Identification of a Conserved Putative Secretion Signal for Type III Secretion Systems. PLoS Pathogens, 2009, 5, e1000375.	4.7	177
40	A generalized knowledgeâ€based discriminatory function for biomolecular interactions. Proteins: Structure, Function and Bioinformatics, 2009, 76, 115-128.	2.6	26
41	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
42	Prediction and Integration of Regulatory and Proteinâ€"Protein Interactions. Methods in Molecular Biology, 2009, 541, 101-143.	0.9	12
43	Inferring Molecular Interactions Pathways from eQTL Data. Methods in Molecular Biology, 2009, 541, 211-223.	0.9	5
44	Diversity of protein structures and difficulties in fold recognition: the curious case of protein G. F1000 Biology Reports, 2009, 1, 69.	4.0	11
45	Improving the accuracy of template-based predictions by mixing and matching between initial models. BMC Structural Biology, 2008, 8, 24.	2.3	13
46	Scoring Functions for De Novo Protein Structure Prediction Revisited. , 2008, 413, 243-281.		10
47	Novel paradigms for drug discovery: computational multitarget screening. Trends in Pharmacological Sciences, 2008, 29, 62-71.	8.7	127
48	Protein Meta-Functional Signatures from Combining Sequence, Structure, Evolution, and Amino Acid Property Information. PLoS Computational Biology, 2008, 4, e1000181.	3.2	37
49	Identification of potential HIV-1 targets of minocycline. Bioinformatics, 2007, 23, 2797-2799.	4.1	18
50	Structural polymorphism and diversifying selection on the pregnancy malaria vaccine candidate VAR2CSA. Molecular and Biochemical Parasitology, 2007, 155, 103-112.	1.1	111
51	De Novo Protein Structure Prediction. Biological and Medical Physics Series, 2007, , 43-63.	0.4	7
52	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
53	Crystal Structure and Mutational Analysis of the DaaE Adhesin of Escherichia coli. Journal of Biological Chemistry, 2006, 281, 22367-22377.	3.4	24
54	Virtual screening of HIV-1 protease inhibitors against human cytomegalovirus protease using docking and molecular dynamics. Aids, 2005, 19, 529-531.	2.2	15

#	Article	IF	Citations
55	The Genomes of Oryza sativa: A History of Duplications. PLoS Biology, 2005, 3, e38.	5.6	808
56	FSSA: a novel method for identifying functional signatures from structural alignments. Bioinformatics, 2005, 21, 2969-2977.	4.1	25
57	Improvement in protein functional site prediction by distinguishing structural and functional constraints on protein family evolution using computational design. Nucleic Acids Research, 2005, 33, 5861-5867.	14.5	78
58	Functional annotation from predicted protein interaction networks. Bioinformatics, 2005, 21, 3217-3226.	4.1	54
59	Identification of Potential Multitarget Antimalarial Drugs. JAMA - Journal of the American Medical Association, 2005, 294, 1487.	7.4	28
60	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
61	PROTINFO: new algorithms for enhanced protein structure predictions. Nucleic Acids Research, 2005, 33, W77-W80.	14.5	60
62	PIRSpred: a web server for reliable HIV-1 protein-inhibitor resistance/susceptibility prediction. Trends in Microbiology, 2005, 13, 150-151.	7.7	21
63	Prediction of HIV-1 protease inhibitor resistance using a protein-inhibitor flexible docking approach. Antiviral Therapy, 2005, 10, 157-66.	1.0	24
64	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
65	Prediction of HIV-1 Protease Inhibitor Resistance using a Proteinâ€"Inhibitor Flexible Docking Approach. Antiviral Therapy, 2005, 10, 157-166.	1.0	40
66	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
67	HIVâ€1 Genotypic Drugâ€Resistance Interpretation Algorithms Need to Include Hypersusceptibilityâ€Associated Mutations. Journal of Infectious Diseases, 2004, 190, 2055-2056.	4.0	8
68	Neutral evolution of â€˜non-codingâ€™ complementary DNAs. Nature, 2004, 431, 1-2.	27.8	127
69	Enhanced functional information from predicted protein networks. Trends in Biotechnology, 2004, 22, 60-62.	9.3	18
70	Improved protein structure selection using decoy-dependent discriminatory functions. BMC Structural Biology, 2004, 4, 8.	2.3	56
71	Improved accuracy of HIV-1 genotypic susceptibility interpretation using a consensus approach. Aids, 2004, 18, 1858-1859.	2.2	12
72	Simple linear model provides highly accurate genotypic predictions of HIV-1 drug resistance. Antiviral Therapy, 2004, 9, 343-52.	1.0	22

#	Article	IF	Citations
73	Simple Linear Model Provides Highly Accurate Genotypic Predictions of HIV-1 Drug Resistance. Antiviral Therapy, 2004, 9, 343-352.	1.0	45
74	Antivirogram or Phenosense: A Comparison of their Reproducibility and an Analysis of their Correlation. Antiviral Therapy, 2004, 9, 703-712.	1.0	15
75	Identifying inhibitors of the SARS coronavirus proteinase. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 3989-3992.	2.2	63
76	Improved prediction of HIV-1 protease-inhibitor binding energies by molecular dynamics simulations. BMC Structural Biology, 2003, 3, 2.	2.3	62
77	Accurate and automated classification of protein secondary structure with PsiCSI. Protein Science, 2003, 12, 288-295.	7.6	44
78	PROTINFO: secondary and tertiary protein structure prediction. Nucleic Acids Research, 2003, 31, 3296-3299.	14.5	38
79	Modeling genome structure and function. Pure and Applied Chemistry, 2002, 74, 907-914.	1.9	2
80	A comprehensive analysis of 40 blind protein structure predictions. , 2002, 2, 3.		47
81	Decoys â€˜Râ€™ Us: A database of incorrect conformations to improve protein structure prediction. Protein Science, 2000, 9, 1399-1401.	7.6	215
82	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
83	Scoring Functions for ab initio Protein Structure Prediction. , 2000, 143, 223-245.		10
84	Ab initio construction of protein tertiary structures using a hierarchical approach. Journal of Molecular Biology, 2000, 300, 171-185.	4.2	162
85	Ab initio protein structure prediction using a combined hierarchical approach. Proteins: Structure, Function and Bioinformatics, 1999, 37, 194-198.	2.6	66
86	Ab Initio fold prediction of small helical proteins using distance geometry and knowledge-based scoring functions 1 1Edited by F. Cohen. Journal of Molecular Biology, 1999, 290, 267-281.	4.2	89
87	Ab initio protein structure prediction using a combined hierarchical approach. Proteins: Structure, Function and Bioinformatics, 1999, 37, 194-198.	2.6	27
88	Probing structure-function relationships of the DNA polymerase alpha-associated zinc-finger protein using computational approaches. , 1999, , 179-90.		1
89	Distance geometry generates nativeâ€“like folds for small helical proteins using the consensus distances of predicted protein structures. Protein Science, 1998, 7, 1998-2003.	7.6	26
90	An all-atom distance-dependent conditional probability discriminatory function for protein structure prediction 1 1Edited by F. Cohen. Journal of Molecular Biology, 1998, 275, 895-916.	4.2	429

#	Article	IF	Citations
91	A graph-theoretic algorithm for comparative modeling of protein structure. Journal of Molecular Biology, 1998, 279, 287-302.	4.2	133
92	A COMBINED APPROACH FOR AB INITIO CONSTRUCTION OF LOW RESOLUTION PROTEIN TERTIARY STRUCTURES FROM SEQUENCE. , 1998, , 505-16.		34
93	Handling context-sensitivity in protein structures using graph theory: Bona fide prediction. Proteins: Structure, Function and Bioinformatics, 1997, 29, 43-49.	2.6	15
94	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