Subbarao Naidu

List of Publications by Year
in descending order

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90 papers	2,311 citations	279798 23 h-index	243625 44 g-index
94 all docs	94 docs citations	94 times ranked	3300 citing authors

#	Article	IF	Citations
1	Discovery of multi-target mur enzymes inhibitors with anti-mycobacterial activity through a Scaffold approach. Journal of Biomolecular Structure and Dynamics, 2023, 41, 2878-2899.	3.5	5
2	In silico identification of small molecule protein-protein interaction inhibitors: targeting hotspot regions at the interface of MXRA8 and CHIKV envelope protein. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3349-3367.	3.5	4
3	In-silico prediction of potential inhibitors against phosphatidylinositol 3-kinase catalytic subunit alpha involved in head and neck squamous cell carcinomas. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4697-4712.	3.5	5
4	Identification of novel multitarget antitubercular inhibitors against mycobacterial peptidoglycan biosynthetic Mur enzymes by structure-based virtual screening. Journal of Biomolecular Structure and Dynamics, 2022, 40, 8185-8196.	3.5	7
5	Exploring the interaction mechanism between potential inhibitor and multi-target Mur enzymes of mycobacterium tuberculosis using molecular docking, molecular dynamics simulation, principal component analysis, free energy landscape, dynamic cross-correlation matrices, vector movements, and binding free energy calculation. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13497-13526.	3.5	20
6	The tetrameric structure of Plasmodium falciparum phosphoglycerate mutase is critical for optimal enzymatic activity. Journal of Biological Chemistry, 2022, 298, 101713.	3.4	0
7	A hybrid resampling algorithms SMOTE and ENN based deep learning models for identification of Marburg virus inhibitors. Future Medicinal Chemistry, 2022, 14, 701-715.	2.3	4
8	In silico identification and in vitro antiviral validation of potential inhibitors against Chikungunya virus. Journal of Computer-Aided Molecular Design, 2022, 36, 521-536.	2.9	2
9	Exploring Molecular Descriptors and Fingerprints to Predict mTOR Kinase Inhibitors using Machine Learning Techniques. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2021, 18, 1902-1913.	3.0	8
10	Designing novel inhibitors against cyclopropane mycolic acid synthase 3 (PcaA): targeting dormant state of Mycobacterium tuberculosis. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6339-6354.	3.5	4
11	A comparative study of human betacoronavirus spike proteins: structure, function and therapeutics. Archives of Virology, 2021, 166, 697-714.	2.1	21
12	Dynamic interaction between lysozyme and ceftazidime: Experimental and molecular simulation approaches. Journal of Molecular Liquids, 2021, 328, 115412.	4.9	32
13	Deep learning model for virtual screening of novel 3C-like protease enzyme inhibitors against SARS coronavirus diseases. Computers in Biology and Medicine, 2021, 132, 104317.	7.0	23
14	Noncovalent molecular interactions between antineoplastic drug gemcitabine and a carrier protein identified through spectroscopic and in silico methods. International Journal of Biological Macromolecules, 2021, 182, 993-1002.	7.5	23
15	New Framework for the Discovery of PRC2 Inhibitors: Epigenetic Drugs. Current Drug Targets, 2021, 22, 1198-1206.	2.1	1
16	Insilico study on the effect of SARS-CoV-2 RBD hotspot mutantsâ€™ interaction with ACE2 to understand the binding affinity and stability. Virology, 2021, 561, 107-116.	2.4	44
17	Current and Future Therapeutic Targets: A Review on Treating Head and Neck Squamous Cell Carcinoma. Current Cancer Drug Targets, 2021, 21, 386-400.	1.6	11
18	Exploring the Molecular Level Interaction of Human Serum Albumin with Calcium Oxalate Monohydrate Crystals. Protein and Peptide Letters, 2021, 28, 1281-1289.	0.9	2

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19	Thermodynamics, molecular modelling and denaturation studies on exploring the binding mechanism of tetramethylpyrazine with human serum albumin. Journal of Chemical Thermodynamics, 2020, 140, 105915.	2.0	15
20	A genetic programming-based approach to identify potential inhibitors of serine protease of Mycobacterium tuberculosis. Future Medicinal Chemistry, 2020, 12, 147-159.	2.3	1
21	Virtual screening to identify novel potential inhibitors for Glutamine synthetase of Mycobacterium tuberculosis. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5062-5080.	3.5	19
22	Envelope proteins as antiviral drug target. Journal of Drug Targeting, 2020, 28, 1046-1052.	4.4	14
23	Using SMOTE to Deal with Class-Imbalance Problem in Bioactivity Data to Predict mTOR Inhibitors. SN Computer Science, 2020, 1, 1.	3.6	8
24	Estimation of a stronger heparin binding locus in fibronectin domain III¹⁴using thermodynamics and molecular dynamics. RSC Advances, 2020, 10, 20288-20301.	3.6	9
25	Design and in vitro analysis of SIRT2 inhibitor targeting Parkinsonâ€™s disease. Molecular Diversity, 2020, 25, 2261-2270.	3.9	7
26	Polycomb repressive complex 2 inhibitors: emerging epigenetic modulators. Drug Discovery Today, 2019, 24, 179-188.	6.4	11
27	Development and rigorous validation of antimalarial predictive models using machine learning approaches. SAR and QSAR in Environmental Research, 2019, 30, 543-560.	2.2	14
28	CID-6033590 inhibits p38MAPK pathway and induces S-phase cell cycle arrest and apoptosis in DU145 and PC-3 cells. Toxicology in Vitro, 2019, 60, 420-436.	2.4	12
29	Enhancement in the Catalytic Activity of Human Salivary Aldehyde Dehydrogenase by Alliin from Garlic: Implications in Aldehyde Toxicity and Oral Health. Current Pharmaceutical Biotechnology, 2019, 20, 506-516.	1.6	7
30	Diagnostic Significance of p38 Isoforms (p38Î±, p38Î², p38Î³, p38Î´) in Head and Neck Squamous Cell Carcinoma: Comparative Serum Level Evaluation and Design of Novel Peptide Inhibitor Targeting the Same. Cancer Research and Treatment, 2019, 51, 313-325.	3.0	15
31	Exploring the Modulatory Effect of Albumin on Calcium Phosphate Crystallization. Current Science, 2019, 117, 1083.	0.8	1
32	Calorimetric, spectroscopic and molecular modelling insight into the interaction of gallic acid with bovine serum albumin. Journal of Chemical Thermodynamics, 2018, 122, 85-94.	2.0	49
33	Identification of novel inhibitors against UDPâ€galactopyranose mutase to combat leishmaniasis. Journal of Cellular Biochemistry, 2018, 119, 2653-2665.	2.6	27
34	In silico study directed towards identification of novel high-affinity inhibitors targeting an oncogenic protein: BRD4-BD1. SAR and QSAR in Environmental Research, 2018, 29, 975-996.	2.2	12
35	Stress-induced nuclear depletion of Entamoeba histolytica 3â€²-5â€² exoribonuclease EhRrp6 and its role in growth and erythrophagocytosis. Journal of Biological Chemistry, 2018, 293, 16242-16260.	3.4	14
36	Molecular Analysis and Modeling of Hepatitis E Virus Helicase and Identification of Novel Inhibitors by Virtual Screening. BioMed Research International, 2018, 2018, 1-8.	1.9	8

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37	Role of tyrosine residue (Y213) in nuclear retention of PCNA1 in human malaria parasite Plasmodium falciparum. FEMS Microbiology Letters, 2018, 365, .	1.8	4
38	In silico identification of inhibitors against Plasmodium falciparum histone deacetylase 1 (PfHDAC-1). Journal of Molecular Modeling, 2018, 24, 232.	1.8	8
39	Designing novel inhibitors against Mycobacterium tuberculosis FadA5 (acetyl-CoA acetyltransferase) by virtual screening of known anti-tuberculosis (bioactive) compounds. Bioinformation, 2018, 14, 327-336.	0.5	6
40	Screening and analysis of acetyl-cholinesterase (AChE) inhibitors in the context of Alzheimerâ€™s disease. Bioinformation, 2018, 14, 414-429.	0.5	8
41	A genetic programming-based approach and machine learning approaches to the classification of multiclass anti-malarial datasets. International Journal of Computational Biology and Drug Design, 2018, 11, 275.	0.3	0
42	Comparative analysis of machine learning based QSAR models and molecular docking studies to screen potential anti-tubercular inhibitors against InhA of mycobacterium tuberculosis. International Journal of Computational Biology and Drug Design, 2018, 11, 209.	0.3	1
43	Allosteric inhibition of topoisomerase I by pinostrobin: Molecular docking, spectroscopic and topoisomerase I activity studies. Journal of Photochemistry and Photobiology B: Biology, 2017, 167, 299-308.	3.8	22
44	In vivo anti-inflammatory activity and docking study of newly synthesized benzimidazole derivatives bearing oxadiazole and morpholine rings. Bioorganic Chemistry, 2017, 70, 107-117.	4.1	52
45	Designing novel inhibitors against histone acetyltransferase (HAT:ÂGCN5) of Plasmodium falciparum. European Journal of Medicinal Chemistry, 2017, 138, 26-37.	5.5	22
46	Analyzing the role of CagV, a VirB8 homolog of the type IV secretion system of Helicobacter pylori. FEBS Open Bio, 2017, 7, 915-933.	2.3	10
47	Designing, synthesis, and antimicrobial action of oxazoline and thiazoline derivatives of fatty acid esters. Journal of Biomolecular Structure and Dynamics, 2017, 35, 3412-3431.	3.5	20
48	Design, synthesis of allosteric peptide activator for human SIRT1 and its biological evaluation in cellular model of Alzheimer's disease. European Journal of Medicinal Chemistry, 2017, 127, 909-916.	5.5	27
49	High Throughput Virtual Screening to Identify Novel natural product Inhibitors for MethionyltRNA-Synthetase of Brucella melitensis. Bioinformation, 2017, 13, 8-16.	0.5	7
50	Evaluation of predictive models based on random forest, decision tree and support vector machine classifiers and virtual screening of anti-mycobacterial compounds. International Journal of Computational Biology and Drug Design, 2017, 10, 248.	0.3	0
51	3D QSAR, pharmacophore and molecular docking studies of known inhibitors and designing of novel inhibitors for M18 aspartyl aminopeptidase of Plasmodium falciparum. BMC Structural Biology, 2016, 16, 12.	2.3	25
52	Docking and molecular dynamics simulation study of EGFR1 with EGF-like peptides to understand molecular interactions. Molecular BioSystems, 2016, 12, 1987-1995.	2.9	11
53	Pharmacophore based virtual screening for identification of marine bioactive compounds as inhibitors against macrophage infectivity potentiator (Mip) protein of Chlamydia trachomatis. RSC Advances, 2016, 6, 18946-18957.	3.6	7
54	Interaction of the recently approved anticancer drug nintedanib with human acute phase reactant Î± 1-acid glycoprotein. Journal of Molecular Structure, 2016, 1115, 171-179.	3.6	13

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55	Transcription regulation of nuclear receptor PXR: Role of SUMO-1 modification and NDSM in receptor function. Molecular and Cellular Endocrinology, 2016, 420, 194-207.	3.2	17
56	Functional dissection of proliferating-cell nuclear antigens (1 and 2) in human malarial parasitePlasmodium falciparum:possible involvement in DNA replication and DNA damage response. Biochemical Journal, 2015, 470, 115-129.	3.7	26
57	Biochemical Analysis of CagE: A VirB4 Homologue of Helicobacter pylori Cag-T4SS. PLoS ONE, 2015, 10, e0142606.	2.5	32
58	In Silico Analysis of Conformational Changes Induced by Normal and Mutation of Macrophage Infectivity Potentiator Catalytic Residues and its Interactions with Rapamycin. Interdisciplinary Sciences, Computational Life Sciences, 2015, 7, 326-333.	3.6	6
59	Biophysical insight into the anti-amyloidogenic behavior of taurine. International Journal of Biological Macromolecules, 2015, 80, 375-384.	7.5	78
60	Interaction of biocompatible natural rosin-based surfactants with human serum albumin: A biophysical study. Journal of Luminescence, 2015, 167, 399-407.	3.1	27
61	In Silico Screening for Novel Inhibitors of DNA Polymerase III Alpha Subunit of Mycobacterium tuberculosis (MtbDnaE2, H37Rv). PLoS ONE, 2015, 10, e0119760.	2.5	15
62	In Silico Screening, Genotyping, Molecular Dynamics Simulation and Activity Studies of SNPs in Pyruvate Kinase M2. PLoS ONE, 2015, 10, e0120469.	2.5	19
63	The Rational Design of Specific Peptide Inhibitor against p38Î± MAPK at Allosteric-Site: A Therapeutic Modality for HNSCC. PLoS ONE, 2014, 9, e101525.	2.5	20
64	Structure-based screening of inhibitors against KPC-2: designing potential drug candidates against multidrug-resistant bacteria. Journal of Biomolecular Structure and Dynamics, 2014, 32, 741-750.	3.5	23
65	Molecular simulation of Tyr105 phosphorylated pyruvate kinase M2 to understand its structure and dynamics. Journal of Molecular Modeling, 2014, 20, 2447.	1.8	8
66	Bacterialâ€induced expression of RAB18 protein in Orzya sativa salinity stress and insights into molecular interaction with GTP ligand. Journal of Molecular Recognition, 2014, 27, 521-527.	2.1	32
67	Insight into the Effect of Inhibitor Resistant S130G Mutant on Physico-Chemical Properties of SHV Type Beta-Lactamase: A Molecular Dynamics Study. PLoS ONE, 2014, 9, e112456.	2.5	56
68	PfalDB: An Integrated Drug Target and Chemical Database for Plasmodium flaciparum. Current Drug Targets, 2014, 15, 1089-1093.	2.1	1
69	Development of peptide inhibitor as a therapeutic agent against head and neck squamous cell carcinoma (HNSCC) targeting p38Î± MAP kinase. Biochimica Et Biophysica Acta - General Subjects, 2013, 1830, 2763-2769.	2.4	17
70	Designing and synthesis of novel antimicrobial heterocyclic analogs of fatty acids. European Journal of Medicinal Chemistry, 2013, 70, 887-900.	5.5	28
71	Biophysical Insight into Furosemide Binding to Human Serum Albumin: A Study To Unveil Its Impaired Albumin Binding in Uremia. Journal of Physical Chemistry B, 2013, 117, 2595-2604.	2.6	104
72	Virtual Screening, Identification and In Vitro Testing of Novel Inhibitors of O-Acetyl-L-Serine Sulfhydrylase of Entamoeba histolytica. PLoS ONE, 2012, 7, e30305.	2.5	62

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73	In-silico modeling of a novel OXA-51 from Î²-lactam-resistant Acinetobacter baumannii and its interaction with various antibiotics. Journal of Molecular Modeling, 2012, 18, 3351-3361.	1.8	34
74	DNA binding activity of Helicobacter pylori DnaB helicase: the role of the Nâ€terminal domain in modulating DNA binding activities. FEBS Journal, 2012, 279, 234-250.	4.7	12
75	Structural studies of serine acetyltransferase 1 fromEntamoeba histolytica. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C352-C353.	0.3	0
76	Mitoxantrone Induced Impediment of Histone Acetylation and Structural Flexibility of the Protein. Cell Biochemistry and Biophysics, 2011, 60, 209-218.	1.8	11
77	Structural and Biochemical Studies of Serine Acetyltransferase Reveal Why the Parasite Entamoeba histolytica Cannot Form a Cysteine Synthase Complex. Journal of Biological Chemistry, 2011, 286, 12533-12541.	3.4	50
78	Elimination of Endogenous Toxin, Creatinine from Blood Plasma Depends on Albumin Conformation: Site Specific Uremic Toxicity & Impaired Drug Binding. PLoS ONE, 2011, 6, e17230.	2.5	108
79	Stereo-Selectivity of Human Serum Albumin to Enantiomeric and Isoelectronic Pollutants Dissected by Spectroscopy, Calorimetry and Bioinformatics. PLoS ONE, 2011, 6, e26186.	2.5	133
80	Homology modelling of a sensor histidine kinase from Aeromonas hydrophila. Journal of Molecular Modeling, 2010, 16, 1003-1009.	1.8	7
81	Ligand binding strategies of human serum albumin: How can the cargo be utilized?. Chirality, 2010, 22, 77-87.	2.6	295
82	Predictive inference on cytoplasmic and mitochondrial thioredoxin peroxidases in the highly radioresistant Lepidopteran insect Spodoptera frugiperda. Bioinformation, 2010, 4, 399-404.	0.5	5
83	Analysis of oligomeric proteins during unfolding by pH and temperature. Journal of Molecular Modeling, 2009, 15, 1013-1025.	1.8	1
84	Identification of novel target sites and an inhibitor of the dengue virus E protein. Journal of Computer-Aided Molecular Design, 2009, 23, 333-341.	2.9	77
85	Molecular modeling on pyruvate phosphate dikinase of Entamoeba histolytica and in silico virtual screening for novel inhibitors. Journal of Computer-Aided Molecular Design, 2008, 22, 647-660.	2.9	16
86	Characterization of doxorubicin binding site and drug induced alteration in the functionally important structural state of oxyhemoglobin. Journal of Pharmaceutical and Biomedical Analysis, 2008, 48, 1096-1104.	2.8	21
87	Interaction of mitoxantrone with human serum albumin: Spectroscopic and molecular modeling studies. European Journal of Pharmaceutical Sciences, 2008, 35, 371-382.	4.0	182
88	In silico Modeling of Î±1A-Adrenoceptor: Interaction of its Normal and Mutated Active Sites with Noradrenaline as well as its Agonist and Antagonist. American Journal of Biochemistry and Biotechnology, 2007, 3, 216-224.	0.4	10
89	A robust and efficient automated docking algorithm for molecular recognition. Protein Engineering, Design and Selection, 1992, 5, 69-75.	2.1	35
90	Defining topologigical equivalences in macromolecules. Protein Engineering, Design and Selection, 1991, 4, 877-884.	2.1	32