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	Ligand binding strategies of human serum albumin: How can the cargo be utilized?. Chirality, 2010, 22, 77-87.	2.6	295
2	Interaction of mitoxantrone with human serum albumin: Spectroscopic and molecular modeling studies. European Journal of Pharmaceutical Sciences, 2008, 35, 371-382.	4.0	182
3	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
4	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
5	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
6	Biophysical insight into the anti-amyloidogenic behavior of taurine. International Journal of Biological Macromolecules, 2015, 80, 375-384.	7.5	78
7	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
8	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
9	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
10	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
11	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
12	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
13	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
14	A robust and efficient automated docking algorithm for molecular recognition. Protein Engineering, Design and Selection, 1992, 5, 69-75.	2.1	35
15	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
16	Defining topologigical equivalences in macromolecules. Protein Engineering, Design and Selection, 1991, 4, 877-884.	2.1	32
17	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
18	Biochemical Analysis of CagE: A VirB4 Homologue of Helicobacter pylori Cag-T4SS. PLoS ONE, 2015, 10, e0142606.	2.5	32

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19	Dynamic interaction between lysozyme and ceftazidime: Experimental and molecular simulation approaches. Journal of Molecular Liquids, 2021, 328, 115412.	4.9	32
20	Designing and synthesis of novel antimicrobial heterocyclic analogs of fatty acids. European Journal of Medicinal Chemistry, 2013, 70, 887-900.	5.5	28
21	Interaction of biocompatible natural rosin-based surfactants with human serum albumin: A biophysical study. Journal of Luminescence, 2015, 167, 399-407.	3.1	27
22	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
23	Identification of novel inhibitors against UDPâ€galactopyranose mutase to combat leishmaniasis. Journal of Cellular Biochemistry, 2018, 119, 2653-2665.	2.6	27
24	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
25	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
26	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
27	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
28	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
29	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
30	Designing novel inhibitors against histone acetyltransferase (HAT:ÂGCN5) of Plasmodium falciparum. European Journal of Medicinal Chemistry, 2017, 138, 26-37.	5.5	22
31	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
32	A comparative study of human betacoronavirus spike proteins: structure, function and therapeutics. Archives of Virology, 2021, 166, 697-714.	2.1	21
33	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
34	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
35	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
36	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

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37	In Silico Screening, Genotyping, Molecular Dynamics Simulation and Activity Studies of SNPs in Pyruvate Kinase M2. PLoS ONE, 2015, 10, e0120469.	2.5	19
38	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
39	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
40	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
41	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
42	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
43	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
44	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
45	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
46	Envelope proteins as antiviral drug target. Journal of Drug Targeting, 2020, 28, 1046-1052.	4.4	14
47	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
48	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
49	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
50	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
51	Mitoxantrone Induced Impediment of Histone Acetylation and Structural Flexibility of the Protein. Cell Biochemistry and Biophysics, 2011, 60, 209-218.	1.8	11
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	Polycomb repressive complex 2 inhibitors: emerging epigenetic modulators. Drug Discovery Today, 2019, 24, 179-188.	6.4	11
54	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

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55	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
56	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
57	Estimation of a stronger heparin binding locus in fibronectin domain III¹⁴using thermodynamics and molecular dynamics. RSC Advances, 2020, 10, 20288-20301.	3.6	9
58	Molecular simulation of Tyr105 phosphorylated pyruvate kinase M2 to understand its structure and dynamics. Journal of Molecular Modeling, 2014, 20, 2447.	1.8	8
59	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
60	In silico identification of inhibitors against Plasmodium falciparum histone deacetylase 1 (PfHDAC-1). Journal of Molecular Modeling, 2018, 24, 232.	1.8	8
61	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
62	Using SMOTE to Deal with Class-Imbalance Problem in Bioactivity Data to Predict mTOR Inhibitors. SN Computer Science, 2020, 1, 1.	3.6	8
63	Screening and analysis of acetyl-cholinesterase (AChE) inhibitors in the context of Alzheimerâ€™s disease. Bioinformation, 2018, 14, 414-429.	0.5	8
64	Homology modelling of a sensor histidine kinase from Aeromonas hydrophila. Journal of Molecular Modeling, 2010, 16, 1003-1009.	1.8	7
65	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
66	Design and in vitro analysis of SIRT2 inhibitor targeting Parkinsonâ€™s disease. Molecular Diversity, 2020, 25, 2261-2270.	3.9	7
67	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
68	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
69	High Throughput Virtual Screening to Identify Novel natural product Inhibitors for MethionyltRNA-Synthetase of Brucella melitensis. Bioinformation, 2017, 13, 8-16.	0.5	7
70	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
71	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
72	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

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73	Predictive inference on cytoplasmic and mitochondrial thioredoxin peroxidases in the highly radioresistant Lepidopteran insect Spodoptera frugiperda. Bioinformation, 2010, 4, 399-404.	0.5	5
74	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
75	Role of tyrosine residue (Y213) in nuclear retention of PCNA1 in human malaria parasite Plasmodium falciparum. FEMS Microbiology Letters, 2018, 365, .	1.8	4
76	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
77	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
78	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
79	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
80	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
81	Analysis of oligomeric proteins during unfolding by pH and temperature. Journal of Molecular Modeling, 2009, 15, 1013-1025.	1.8	1
82	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
83	New Framework for the Discovery of PRC2 Inhibitors: Epigenetic Drugs. Current Drug Targets, 2021, 22, 1198-1206.	2.1	1
84	PfalDB: An Integrated Drug Target and Chemical Database for Plasmodium flaciparum. Current Drug Targets, 2014, 15, 1089-1093.	2.1	1
85	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
86	Exploring the Modulatory Effect of Albumin on Calcium Phosphate Crystallization. Current Science, 2019, 117, 1083.	0.8	1
87	Structural studies of serine acetyltransferase 1 fromEntamoeba histolytica. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C352-C353.	0.3	0
88	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
89	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
90	The tetrameric structure of Plasmodium falciparum phosphoglycerate mutase is critical for optimal enzymatic activity. Journal of Biological Chemistry, 2022, 298, 101713.	3.4	0