Sanjeev Kumar Singh

List of Publications by Year
in descending order

186	3,876	147566	214527
papers	citations	31 h-index	47 g-index

192	192	192	3664
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Targeting COVID-19 (SARS-CoV-2) main protease through active phytochemicals of ayurvedic medicinal plants â€“ Withania somnifera (Ashwagandha), Tinospora cordifolia (Giloy) and Ocimum sanctum (Tulsi) â€“ a molecular docking study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 190-203.	2.0	181
2	Extra precision docking, free energy calculation and molecular dynamics simulation studies of CDK2 inhibitors. Journal of Theoretical Biology, 2013, 334, 87-100.	0.8	155
3	Identification of new anti-nCoV drug chemical compounds from Indian spices exploiting SARS-CoV-2 main protease as target. Journal of Biomolecular Structure and Dynamics, 2020, , 1-9.	2.0	132
4	Hydroxychloroquine Inhibits Zika Virus NS2B-NS3 Protease. ACS Omega, 2018, 3, 18132-18141.	1.6	86
5	Epigallocatechin gallate, an active green tea compound inhibits the Zika virus entry into host cells via binding the envelope protein. International Journal of Biological Macromolecules, 2017, 104, 1046-1054.	3.6	84
6	Bioremediation of multi-metal contaminated soil using biosurfactant â€” a novel approach. Indian Journal of Microbiology, 2008, 48, 142-146.	1.5	81
7	Constitutive Inflammatory Cytokine Storm: A Major Threat to Human Health. Journal of Interferon and Cytokine Research, 2020, 40, 19-23.	0.5	78
8	Structure-based virtual screening and molecular dynamics simulation of SARS-CoV-2 Guanine-N7 methyltransferase (nsp14) for identifying antiviral inhibitors against COVID-19. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4582-4593.	2.0	73
9	Î²-Sitosterol targets Trx/Trx1 reductase to induce apoptosis in A549 cells via ROS mediated mitochondrial dysregulation and p53 activation. Scientific Reports, 2018, 8, 2071.	1.6	71
10	Screening, isolation and characterization of biosurfactant producing Bacillus subtilis strain ANSKLAB03. Bioinformation, 2018, 14, 304-314.	0.2	71
11	Effect of biosludge and biofertilizer amendment on growth of Jatropha curcas in heavy metal contaminated soils. Environmental Monitoring and Assessment, 2008, 145, 7-15.	1.3	65
12	Novel ligand-based docking; molecular dynamic simulations; and absorption, distribution, metabolism, and excretion approach to analyzing potential acetylcholinesterase inhibitors for Alzheimer's disease. Journal of Pharmaceutical Analysis, 2018, 8, 413-420.	2.4	46
13	Vitexin inhibits AÎ²25-35 induced toxicity in Neuro-2a cells by augmenting Nrf-2/HO-1 dependent antioxidant pathway and regulating lipid homeostasis by the activation of LXR-Î±. Toxicology in Vitro, 2018, 50, 160-171.	1.1	42
14	3D-QSAR CoMFA study onÂindenopyrazole derivatives asÂcyclin dependent kinase 4 (CDK4) andÂcyclin dependent kinase 2 (CDK2) inhibitors. European Journal of Medicinal Chemistry, 2006, 41, 1310-1319.	2.6	41
15	In silico and in vitro studies of cinnamaldehyde and their derivatives against LuxS in Streptococcus pyogenes: effects on biofilm and virulence genes. Journal of Molecular Recognition, 2014, 27, 106-116.	1.1	41
16	Assessment of dual inhibition property of newly discovered inhibitors against PCAF and GCN5 throughin silicoscreening, molecular dynamics simulation and DFT approach. Journal of Receptor and Signal Transduction Research, 2015, 35, 370-380.	1.3	41
17	Structural insights into the binding mode of flavonols with the active site of matrix metalloproteinase-9 through molecular docking and molecular dynamic simulations studies. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3718-3739.	2.0	41
18	Exploring the selectivity of a ligand complex with CDK2/CDK1: a molecular dynamics simulation approach. Journal of Molecular Recognition, 2012, 25, 504-512.	1.1	39

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19	Exploration of the binding of DNA binding ligands toStaphylococcalDNA through QM/MM docking and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2013, 31, 561-571.	2.0	38
20	In Silico and In Vitro Studies on the Protein-Protein Interactions between Brugia malayi Immunomodulatory Protein Calreticulin and Human C1q. PLoS ONE, 2014, 9, e106413.	1.1	38
21	Atom-based 3D-QSAR, molecular docking, DFT, and simulation studies of acylhydrazone, hydrazine, and diazene derivatives as IN-LEDGF/p75 inhibitors. Structural Chemistry, 2021, 32, 337-352.	1.0	38
22	Structure-Based Virtual Screening for the Identification of High Affinity Compounds as Potent VEGFR2 Inhibitors for the Treatment of Renal Cell Carcinoma. Current Topics in Medicinal Chemistry, 2019, 18, 2174-2185.	1.0	38
23	Anti-amyloidogenic and anti-apoptotic effect of Î±-bisabolol against AÎ² induced neurotoxicity in PC12 cells. European Journal of Medicinal Chemistry, 2018, 143, 1196-1207.	2.6	37
24	Validation of potential inhibitors for SrtA againstBacillus anthracisby combined approach of ligand-based and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1333-1349.	2.0	35
25	Insights into the structural basis of 3,5-diaminoindazoles as CDK2 inhibitors: prediction of binding modes and potency by QMâ€“MM interaction, MESP and MD simulation. Molecular BioSystems, 2014, 10, 2189.	2.9	35
26	Structure-based virtual screening toward the discovery of novel inhibitors for impeding the protein-protein interaction between HIV-1 integrase and human lens epithelium-derived growth factor (LEDGF/p75). Journal of Biomolecular Structure and Dynamics, 2018, 36, 3199-3217.	2.0	35
27	Artificial intelligence and machine learning approaches for drug design: challenges and opportunities for the pharmaceutical industries. Molecular Diversity, 2022, 26, 1893-1913.	2.1	35
28	A leishmaniasis study: Structure-based screening and molecular dynamics mechanistic analysis for discovering potent inhibitors of spermidine synthase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2012, 1824, 1476-1483.	1.1	34
29	Molecular insights of protein contour recognition with ligand pharmacophoric sites through combinatorial library design and MD simulation in validating HTLV-1 PR inhibitors. Molecular BioSystems, 2015, 11, 178-189.	2.9	34
30	Molecular dynamic simulations reveal suboptimal binding of salbutamol in T164I variant of Î²2 adrenergic receptor. PLoS ONE, 2017, 12, e0186666.	1.1	34
31	In silico screening of indinavir-based compounds targeting proteolytic activity in HIV PR: binding pocket fit approach. Medicinal Chemistry Research, 2012, 21, 4060-4068.	1.1	33
32	Pharmacophore modelling and atom-based 3D-QSAR studies on N-methyl pyrimidones as HIV-1 integrase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2012, 27, 339-347.	2.5	33
33	Identification of potential HIV-1 integrase strand transfer inhibitors:In silicovirtual screening and QM/MM docking studies. SAR and QSAR in Environmental Research, 2013, 24, 581-595.	1.0	33
34	Virtual Screening Approaches in Identification of Bioactive Compounds Akin to Delphinidin as Potential HER2 Inhibitors for the Treatment of Breast Cancer. Asian Pacific Journal of Cancer Prevention, 2016, 17, 2291-2295.	0.5	33
35	Shape and pharmacophore-based virtual screening to identify potential cytochrome P450 sterol 14Î±-demethylase inhibitors. Journal of Receptor and Signal Transduction Research, 2013, 33, 234-243.	1.3	32
36	Blocking the interaction between HIV-1 integrase and human LEDGF/p75: mutational studies, virtual screening and molecular dynamics simulations. Molecular BioSystems, 2014, 10, 526.	2.9	32

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37	Microsecond MD Simulation and Multiple-Conformation Virtual Screening to Identify Potential Anti-COVID-19 Inhibitors Against SARS-CoV-2 Main Protease. Frontiers in Chemistry, 2020, 8, 595273.	1.8	32
38	Artificial Intelligence, Big Data and Machine Learning Approaches in Precision Medicine & Drug Discovery. Current Drug Targets, 2021, 22, 631-655.	1.0	32
39	Targeting multidrug resistant Mycobacterium tuberculosis htra2 with identical chemical entities of fluoroquinolones. Indian Journal of Pharmaceutical Sciences, 2012, 74, 217.	1.0	32
40	Structural insights into the binding mode of d-sorbitol with sorbitol dehydrogenase using QM-polarized ligand docking and molecular dynamics simulations. Biochemical Engineering Journal, 2016, 114, 244-256.	1.8	31
41	A Virtual Screening Approach for the Identification of High Affinity Small Molecules Targeting BCR-ABL1 Inhibitors for the Treatment of Chronic Myeloid Leukemia. Current Topics in Medicinal Chemistry, 2017, 17, 2989-2996.	1.0	31
42	Biochemical changes in plant leaves as a biomarker of pollution due to anthropogenic activity. Environmental Monitoring and Assessment, 2011, 177, 527-535.	1.3	30
43	E7 oncoprotein of human papillomavirus: Structural dynamics and inhibitor screening study. Gene, 2018, 658, 159-177.	1.0	30
44	Combining in silico and in vitro approaches to identification of potent inhibitor against phospholipase A2 (PLA2). International Journal of Biological Macromolecules, 2020, 144, 53-66.	3.6	30
45	Combined ligand and structure-based approaches on HIV-1 integrase strand transfer inhibitors. Chemico-Biological Interactions, 2014, 218, 71-81.	1.7	29
46	Molecular docking, QPLD, and ADME prediction studies on HIV-1 integrase leads. Medicinal Chemistry Research, 2012, 21, 4239-4251.	1.1	28
47	Exploration of fluoroquinolone resistance in Streptococcus pyogenes: comparative structure analysis of wildâ€type and mutant DNA gyrase. Journal of Molecular Recognition, 2013, 26, 276-285.	1.1	28
48	In Vitro and In Silico Studies of Chitin and Chitosan Based Nanocarriers for Curcumin and Insulin Delivery. Journal of Polymers and the Environment, 2018, 26, 4095-4113.	2.4	28
49	Molecular docking and molecular dynamics simulation studies to identify potent AURKA inhibitors: assessing the performance of density functional theory, MM-GBSA and mass action kinetics calculations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4325-4335.	2.0	28
50	Shape-based Machine Learning Models for the Potential Novel COVID-19 Protease Inhibitors Assisted by Molecular Dynamics Simulation. Current Topics in Medicinal Chemistry, 2020, 20, 2146-2167.	1.0	28
51	Design of novel JAK3 Inhibitors towards Rheumatoid Arthritis using molecular docking analysis. Bioinformation, 2019, 15, 68-78.	0.2	27
52	Molecular docking and structure-based virtual screening studies of potential drug target, CAAX prenyl proteases, ofLeishmania donovani. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2367-2386.	2.0	26
53	Synthesis, antibacterial studies, and molecular modeling studies of 3,4-dihydropyrimidinone compounds. Journal of Chemical Biology, 2016, 9, 31-40.	2.2	26
54	Dihydroactinidiolide, a natural product against Aî²25-35 induced toxicity in Neuro2a cells: Synthesis, in silico and in vitro studies. Bioorganic Chemistry, 2018, 81, 340-349.	2.0	26

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55	Investigating into the molecular interactions of flavonoids targeting NS2B-NS3 protease from ZIKA virus through in-silico approaches. Journal of Biomolecular Structure and Dynamics, 2021, 39, 272-284.	2.0	26
56	An In Silico Investigation of Potential EGFR Inhibitors for the Clinical Treatment of Colorectal Cancer. Current Topics in Medicinal Chemistry, 2019, 18, 2355-2366.	1.0	26
57	An In silico Approach to Identify High Affinity Small Molecule Targeting m-TOR Inhibitors for the Clinical Treatment of Breast Cancer. Asian Pacific Journal of Cancer Prevention, 2019, 20, 1229-1241.	0.5	26
58	Structure-Based Virtual Screening and Biological Evaluation of a Calpain Inhibitor for Prevention of Selenite-Induced Cataractogenesis in an in Vitro System. Journal of Chemical Information and Modeling, 2015, 55, 1686-1697.	2.5	25
59	Mechanistic Insights into Zika Virus NS3 Helicase Inhibition by Epigallocatechin-3-Gallate. ACS Omega, 2020, 5, 11217-11226.	1.6	25
60	Structure-based Virtual Screening for the Identification of High-affinity Small Molecule Towards STAT3 for the Clinical Treatment of Osteosarcoma. Current Topics in Medicinal Chemistry, 2019, 18, 2511-2526.	1.0	25
61	Design of PD-L1 inhibitors for lung cancer. Bioinformation, 2019, 15, 139-150.	0.2	25
62	Comparative structural analysis of two proteins belonging to quorum sensing system inVibrio cholerae. Journal of Biomolecular Structure and Dynamics, 2012, 30, 574-584.	2.0	24
63	Structural elucidation of SrtA enzyme in Enterococcus faecalis: an emphasis on screening of potential inhibitors against the biofilm formation. Molecular BioSystems, 2014, 10, 1775-1789.	2.9	24
64	FLT3 inhibitor design using molecular docking based virtual screening for acute myeloid leukemia. Bioinformation, 2019, 15, 104-115.	0.2	24
65	Virtual Screening of IL-6 Inhibitors for Idiopathic Arthritis. Bioinformation, 2019, 15, 121-130.	0.2	24
66	Screening, isolation and characterization of biosurfactant-producing Bacillus tequilensis strain ANSKLAB04 from brackish river water. International Journal of Environmental Science and Technology, 2019, 16, 7103-7112.	1.8	23
67	Identification of Small Molecule as a High Affinity Î²2 Agonist Promiscuously Targeting Wild and Mutated (Thr164Ile) Î² 2 Adrenergic Receptor in the Treatment of Bronchial Asthma. Current Pharmaceutical Design, 2016, 22, 5221-5233.	0.9	23
68	Advantages of Structure-Based Drug Design Approaches in Neurological Disorders. Current Neuropharmacology, 2017, 15, 1136-1155.	1.4	23
69	Molecular insights on analogs of HIV PR inhibitors toward HTLVâ€1 PR through QM/MM interactions and molecular dynamics studies: comparative structure analysis of wild and mutant HTLVâ€1 PR. Journal of Molecular Recognition, 2014, 27, 696-706.	1.1	22
70	Structure-Based Virtual Screening Reveals Ibrutinib and Zanubrutinib as Potential Repurposed Drugs against COVID-19. International Journal of Molecular Sciences, 2021, 22, 7071.	1.8	22
71	Helix-Coil Transition Signatures B-Raf V600E Mutation and Virtual Screening for Inhibitors Directed Against Mutant B-Raf. Current Drug Metabolism, 2017, 18, 527-534.	0.7	22
72	3D-QSAR CoMFA Study on Oxindole Derivatives as Cyclin Dependent Kinase 1 (CDK1) and Cyclin Dependent Kinase 2 (CDK2) Inhibitors. Medicinal Chemistry, 2007, 3, 75-84.	0.7	21

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73	Examine the characterization of biofilm formation and inhibition by targeting SrtA mechanism in Bacillus subtilis: a combined experimental and theoretical study. Journal of Molecular Modeling, 2014, 20, 2364.	0.8	20
74	Microbe-assisted phytoremediation approach for ecological restoration of zinc mine spoil dump. International Journal of Environment and Pollution, 2010, 43, 236.	0.2	19
75	An in silico pharmacological approach toward the discovery of potent inhibitors to combat drug resistance HIVâ€1 protease variants. Journal of Cellular Biochemistry, 2019, 120, 9063-9081.	1.2	19
76	Computer-aided Drug Designing for the Identification of High-Affinity Small Molecule Targeting CD20 for the Clinical Treatment of Chronic Lymphocytic Leukemia (CLL). Current Topics in Medicinal Chemistry, 2019, 18, 2527-2542.	1.0	19
77	Identification of High-affinity Small Molecules Targeting Gamma Secretase for the Treatment of Alzheimerâ€™s Disease. Current Topics in Medicinal Chemistry, 2019, 19, 1173-1187.	1.0	19
78	A database for the predicted pharmacophoric features of medicinal compounds. Bioinformation, 2011, 6, 167-168.	0.2	19
79	Identification of High-Affinity Small Molecule Targeting IDH2 for the Clinical Treatment of Acute Myeloid Leukemia. Asian Pacific Journal of Cancer Prevention, 2019, 20, 2287-2297.	0.5	19
80	Functional Inhibition of VEGF and EGFR Suppressors in Cancer Treatment. Current Topics in Medicinal Chemistry, 2019, 19, 178-179.	1.0	18
81	Bacterial protein azurin and derived peptides as potential anti-SARS-CoV-2 agents: insights from molecular docking and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5706-5721.	2.0	18
82	Cdk5: A main culprit in neurodegeneration. International Journal of Neuroscience, 2019, 129, 1192-1197.	0.8	17
83	Î±-bisabolol Î²-D-fucopyranoside as a potential modulator of Î²-amyloid peptide induced neurotoxicity: An in vitro & in silico study. Bioorganic Chemistry, 2019, 88, 102935.	2.0	17
84	High-Throughput Screening and Quantum Mechanics for Identifying Potent Inhibitors Against Mac1 Domain of SARS-CoV-2 Nsp3. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2021, 18, 1262-1270.	1.9	17
85	Discovery of Potent Inhibitors for the Inhibition of Dengue Envelope Protein: An In Silico Approach. Current Topics in Medicinal Chemistry, 2018, 18, 1585-1602.	1.0	17
86	Molecular modeling studies and comparative analysis on structurally similar HTLV and HIV protease using HIV-PR inhibitors. Journal of Receptor and Signal Transduction Research, 2014, 34, 361-371.	1.3	16
87	In silico virtual screening of potent inhibitor to hamper the interaction between HIV-1 integrase and LEDGF/p75 interaction using E-pharmacophore modeling, molecular docking, and dynamics simulations. Computational Biology and Chemistry, 2021, 93, 107509.	1.1	16
88	A Computer - Aided Drug Designing for Pharmacological Inhibition of Mutant ALK for the Treatment of Non-small Cell Lung Cancer. Current Topics in Medicinal Chemistry, 2019, 19, 1129-1144.	1.0	16
89	Homology modeling, active site prediction, and targeting the anti hypertension activity through molecular docking on endothelin â€“ B receptor domain. Bioinformation, 2012, 8, 81-86.	0.2	16
90	Mechanistic insights of SrtAâ€“LPXTG blockers targeting the transpeptidase mechanism in Streptococcus mutans. RSC Advances, 2015, 5, 100498-100510.	1.7	15

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91	Structural dynamic studies on identification of EGCG analogues for the inhibition of Human Papillomavirus E7. Scientific Reports, 2020, 10, 8661.	1.6	15
92	3D-QSAR CoMFA and CoMSIA Study on Benzodipyrazoles as Cyclin Dependent Kinase 2 Inhibitors. Medicinal Chemistry, 2008, 4, 313-321.	0.7	14
93	A three-dimensional chemical phase pharmacophore mapping, QSAR modelling and electronic feature analysis of benzofuran salicylic acid derivatives as LYP inhibitors. SAR and QSAR in Environmental Research, 2013, 24, 1025-1040.	1.0	14
94	Virtual screening based on pharmacophoric features of known calpain inhibitors to identify potent inhibitors of calpain. Medicinal Chemistry Research, 2014, 23, 2445-2455.	1.1	14
95	Virtual screening of LPXTG competitive SrtA inhibitors targeting signal transduction mechanism inBacillus anthracis: a combined experimental and theoretical study. Journal of Receptor and Signal Transduction Research, 2014, 34, 221-232.	1.3	14
96	In Silico Insights on GD2 : A Potential Target for Pediatric Neuroblastoma. Current Topics in Medicinal Chemistry, 2020, 19, 2766-2781.	1.0	14
97	Daucosterol disturbs redox homeostasis and elicits oxidative-stress mediated apoptosis in A549â€cells via targeting thioredoxin reductase by a p53 dependent mechanism. European Journal of Pharmacology, 2019, 855, 112-123.	1.7	13
98	Analysis of biosurfactants produced by bacteria growing on textile sludge and their toxicity evaluation for environmental application. Journal of Dispersion Science and Technology, 2020, 41, 510-522.	1.3	13
99	An Overview on Zika Virus and the Importance of Computational Drug Discovery. Journal of Exploratory Research in Pharmacology, 2018, 3, 43-51.	0.2	13
100	Current Computational Approaches for the Development of Anti-HIV Inhibitors: An Overview. Current Pharmaceutical Design, 2019, 25, 3390-3405.	0.9	13
101	In silico Insights on IL-6: A Potential Target for Multicentric Castleman Disease. Current Computer-Aided Drug Design, 2020, 16, 641-653.	0.8	13
102	Utilisation of municipal solid waste as an amendment for reclamation of coal mine spoil dump. International Journal of Environmental Technology and Management, 2007, 7, 407.	0.1	12
103	3D-QSAR CoMFA Study on Aminothiazole Derivatives as Cyclin-Dependent Kinase 2 Inhibitors. QSAR and Combinatorial Science, 2007, 26, 85-91.	1.5	12
104	Homology modeling, molecular dynamics, and docking studies of pattern-recognition transmembrane protein-lipopolysaccharide and Î²-1,3 glucan-binding protein fromFenneropenaeus indicus. Journal of Biomolecular Structure and Dynamics, 2015, 33, 1269-1280.	2.0	12
105	Exploration of cell cycle regulation and modulation of the DNA methylation mechanism of pelargonidin: Insights from the molecular modeling approach. Computational Biology and Chemistry, 2017, 70, 175-185.	1.1	12
106	Identification of Novel Pancreatic Lipase Inhibitors UsingIn SilicoStudies. Endocrine, Metabolic and Immune Disorders - Drug Targets, 2019, 19, 449-457.	0.6	12
107	Investigations on the Interactions of Î»Phage-Derived Peptides Against the SrtA Mechanism in Bacillus anthracis. Applied Biochemistry and Biotechnology, 2014, 172, 1790-1806.	1.4	11
108	Targeting the cyclin-binding groove site to inhibit the catalytic activity of CDK2/cyclin A complex using p27KIP1-derived peptidomimetic inhibitors. Journal of Chemical Biology, 2015, 8, 11-24.	2.2	11

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109	Investigating the folding pathway and substrate induced conformational changes in B. malayi Guanylate kinase. International Journal of Biological Macromolecules, 2017, 94, 621-633.	3.6	11
110	E-pharmacophore-based screening of mGluR5 negative allosteric modulators for central nervous system disorder. Computational Biology and Chemistry, 2019, 78, 414-423.	1.1	11
111	Targeting the NTPase site of Zika virus NS3 helicase for inhibitor discovery. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4827-4837.	2.0	11
112	Spectroscopic and molecular docking studies for the binding and interaction aspects of curcumin-cysteine conjugate and rosmarinic acid with human telomeric G-quadruplex DNA. International Journal of Biological Macromolecules, 2021, 182, 1463-1472.	3.6	11
113	Cyclin Dependent Kinase as Significant Target for Cancer Treatment. Current Cancer Therapy Reviews, 2012, 8, 225-235.	0.2	10
114	Atom-based 3D-QSAR, induced fit docking, and molecular dynamics simulations study of thieno[2,3-b]pyridines negative allosteric modulators of mGluR5. Journal of Receptor and Signal Transduction Research, 2018, 38, 225-239.	1.3	10
115	Understanding the biological role of PqqB in Pseudomonas stutzeri using molecular dynamics simulation approach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4237-4249.	2.0	10
116	Structural Insights into the Molecular Design of ROS1 Inhibitor for the Treatment of Non-Small Cell Lung Cancer (NSCLC). Current Computer-Aided Drug Design, 2021, 17, 387-401.	0.8	10
117	Identification of Potent VEGF Inhibitors for the Clinical Treatment of Glioblastoma, A Virtual Screening Approach. Asian Pacific Journal of Cancer Prevention, 2019, 20, 2681-2692.	0.5	10
118	Comparative Analysis of Various Electrostatic Potentials on Docking Precision Against Cyclinâ€Ðependent Kinase 2 Protein: A Multiple Docking Approach. Chemical Biology and Drug Design, 2015, 85, 107-118.	1.5	9
119	Investigating the Conformational Structure and Potential Site Interactions of SOD Inhibitors on Ec-SOD in Marine Mud Crab Scylla serrata: A Molecular Modeling Approach. Interdisciplinary Sciences, Computational Life Sciences, 2016, 8, 312-318.	2.2	9
120	Interaction investigations of crustacean Î²â€GBP recognition toward pathogenic microbial cell membrane and stimulate upon prophenoloxidase activation. Journal of Molecular Recognition, 2014, 27, 173-183.	1.1	8
121	Insight into the Binding Mode between N-Methyl Pyrimidones and Prototype Foamy Virus Integrase-DNA Complex by QM-Polarized Ligand Docking and Molecular Dynamics Simulations. Current Topics in Medicinal Chemistry, 2015, 15, 43-49.	1.0	8
122	Molecular modeling and structural analysis of nAChR variants uncovers the mechanism of resistance to snake toxins. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1654-1671.	2.0	8
123	De Novo Design of Ligands Using Computational Methods. Methods in Molecular Biology, 2018, 1762, 71-86.	0.4	8
124	In-silico strategies for identification of potent inhibitor for MMP-1 to prevent metastasis of breast cancer. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-20.	2.0	8
125	Structure-Based Virtual Screening, Molecular Docking, and Molecular Dynamics Simulation of VEGF inhibitors for the clinical treatment of Ovarian Cancer. Journal of Molecular Modeling, 2022, 28, 100.	0.8	8
126	Exploration of proteinâ€“protein interaction effects on Î±-2-macroglobulin in an inhibition of serine protease through gene expression and molecular simulations studies. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1841-1854.	2.0	7

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127	Modeling of macromolecular proteins in prophenoloxidase cascade through experimental and computational approaches. Biotechnology and Applied Biochemistry, 2016, 63, 779-788.	1.4	7
128	Structure based identification and biological evaluation of novel and potent inhibitors of PCAF catalytic domain. International Journal of Biological Macromolecules, 2018, 120, 823-834.	3.6	7
129	Interpretations on the Interaction between Protein Tyrosine Phosphatase and E7 Oncoproteins of High and Low-Risk HPV: A Computational Perception. ACS Omega, 2021, 6, 16472-16487.	1.6	7
130	Ion Channels as Therapeutic Targets for Type 1 Diabetes Mellitus. Current Drug Targets, 2020, 21, 132-147.	1.0	7
131	In silico identification of natural product inhibitors against Octamer-binding transcription factor 4 (Oct4) to impede the mechanism of glioma stem cells. PLoS ONE, 2021, 16, e0255803.	1.1	7
132	Ligand-based pharmacophore modelling and screening of DNA minor groove binders targetingStaphylococcus aureus. Journal of Molecular Recognition, 2014, 27, 429-437.	1.1	6
133	Natural vs. reclaimed forests â€“ a case study of successional change, reclamation technique and phytodiversity. International Journal of Mining, Reclamation and Environment, 2015, 29, 476-498.	1.2	6
134	In vitro and in silico studies on cell adhesion protein peroxinectin from Fenneropenaeus indicus and screening of heme blockers against activity. Journal of Molecular Recognition, 2016, 29, 186-198.	1.1	6
135	Evaluation of CAAX prenyl protease II of Leishmania donovani as potential drug target: Infectivity and growth of the parasite is significantly lowered after the gene knockout. European Journal of Pharmaceutical Sciences, 2017, 102, 156-160.	1.9	6
136	Chemopreventive effect of saponin isolated from Gymnema sylevestre on prostate cancer through in silico and in vivo analysis. Medicinal Chemistry Research, 2017, 26, 1915-1925.	1.1	6
137	Exploring the Biology and Structural Architecture of Sortase Role on Biofilm Formation in Gram Positive Pathogens. Current Topics in Medicinal Chemistry, 2019, 18, 2462-2480.	1.0	6
138	Functional insights by comparison of modeled structures of 18kDa small heat shock protein and its mutant in Mycobacterium leprae. Bioinformation, 2008, 3, 230-234.	0.2	6
139	Structure-Based Virtual Screening, Molecular Docking, Molecular Dynamics Simulation and Pharmacokinetic modelling of Cyclooxygenase-2 (COX-2) inhibitor for the clinical treatment of Colorectal Cancer. Molecular Simulation, 2022, 48, 1081-1101.	0.9	6
140	Communication of Î³ Phage Lysin plyG Enzymes Binding toward SrtA for Inhibition ofBacillus Anthracis: Proteinâ€“Protein Interaction and Molecular Dynamics Study. Cell Communication and Adhesion, 2014, 21, 257-265.	1.0	5
141	Unravelling novel congeners from acetyllysine mimicking ligand targeting a lysine acetyltransferase PCAF bromodomain. Journal of Biomolecular Structure and Dynamics, 2018, 36, 4303-4319.	2.0	5
142	Competitive Inhibition of Quercetin and Apigenin at the ATP Binding site of D-Alanine-D-Alanine Ligase of Helicobacter pylori â€“ A Molecular Modeling Approach. Current Biotechnology, 2019, 7, 340-348.	0.2	5
143	Energetically optimized pharmacophore modeling to identify dual negative allosteric modulators against group I mGluRs in neurodegenerative diseases. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2326-2337.	2.0	5
144	Structural insights of macromolecules involved in bacteria-induced apoptosis in the pathogenesis of human diseases. Advances in Protein Chemistry and Structural Biology, 2021, 126, 1-38.	1.0	5

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145	Interrogation of Bacillus anthracis SrtA active site loop forming open/close lid conformations through extensive MD simulations for understanding binding selectivity of SrtA inhibitors. Saudi Journal of Biological Sciences, 2021, 28, 3650-3659.	1.8	5
146	Exploration of New and Potent Lead Molecules Against CAAX Prenyl Protease I of Leishmania donovani Through Pharmacophore Based Virtual Screening Approach. Combinatorial Chemistry and High Throughput Screening, 2017, 20, 255-271.	0.6	5
147	Effect of HIV-1 Subtype C integrase mutations implied using molecular modeling and docking data. Bioinformation, 2016, 12, 221-230.	0.2	5
148	Structure and chemistry of enzymatic active sites that play a role in the switch and conformation mechanism. Advances in Protein Chemistry and Structural Biology, 2022, 130, 59-83.	1.0	5
149	Integrated Transcriptome Profiling Identifies Prognostic Hub Genes as Therapeutic Targets of Glioblastoma: Evidenced by Bioinformatics Analysis. ACS Omega, 2022, 7, 22531-22550.	1.6	5
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