Sanjeev Kumar Singh

List of Publications by Citations

181 papers	2,592 citations	26 h-index	37 g-index
192 ext. papers	3,194 ext. citations	3.1 avg, IF	5.9 L-index

#	Paper	IF	Citations
181	Extra precision docking, free energy calculation and molecular dynamics simulation studies of CDK2 inhibitors. *Journal of Theoretical Biology*, **2013**, 334, 87-100	2.3	119
180	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	3.6	88
179	Targeting COVID-19 (SARS-CoV-2) main protease through active phytochemicals of ayurvedic medicinal plants - (Ashwagandha), (Giloy) and (Tulsi) - a molecular docking study. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-14	3.6	83
178	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	7.9	65
177	Bioremediation of multi-metal contaminated soil using biosurfactant - a novel approach. *Indian Journal of Microbiology*, **2008**, 48, 142-6	3.7	59
176	Hydroxychloroquine Inhibits Zika Virus NS2B-NS3 Protease. *ACS Omega*, **2018**, 3, 18132-18141	3.9	57
175	Effect of biosludge and biofertilizer amendment on growth of Jatropha curcas in heavy metal contaminated soils. *Environmental Monitoring and Assessment*, **2008**, 145, 7-15	3.1	50
174	Sitosterol targets Trx/Trx1 reductase to induce apoptosis in A549 cells via ROS mediated mitochondrial dysregulation and p53 activation. *Scientific Reports*, **2018**, 8, 2071	4.9	44
173	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	3.6	41
172	Constitutive Inflammatory Cytokine Storm: A Major Threat to Human Health. *Journal of Interferon and Cytokine Research*, **2020**, 40, 19-23	3.5	39
171	Screening, isolation and characterization of biosurfactant producing strain ANSKLAB03. *Bioinformation*, **2018**, 14, 304-314	1.1	35
170	Insights into the structural basis of 3,5-diaminoindazoles as CDK2 inhibitors: prediction of binding modes and potency by QM-MM interaction, MESP and MD simulation. *Molecular BioSystems*, **2014**, 10, 2189-201		34
169	3D-QSAR CoMFA study on indenopyrazole derivatives as cyclin dependent kinase 4 (CDK4) and cyclin dependent kinase 2 (CDK2) inhibitors. *European Journal of Medicinal Chemistry*, **2006**, 41, 1310-9	6.8	34
168	Assessment of dual inhibition property of newly discovered inhibitors against PCAF and GCN5 through in silico screening, molecular dynamics simulation and DFT approach. *Journal of Receptor and Signal Transduction Research*, **2015**, 35, 370-80	2.6	33
167	Vitexin inhibits A induced toxicity in Neuro-2a cells by augmenting Nrf-2/HO-1 dependent antioxidant pathway and regulating lipid homeostasis by the activation of LXR- *Toxicology in Vitro* , **2018**, 50, 160-171	3.6	33
166	Exploring the selectivity of a ligand complex with CDK2/CDK1: a molecular dynamics simulation approach. *Journal of Molecular Recognition*, **2012**, 25, 504-12	2.6	31
165	Validation of potential inhibitors for SrtA against Bacillus anthracis by combined approach of ligand-based and molecular dynamics simulation. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 1333-49	3.6	30

164	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, 106-16	2.6	30
163	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	3.6	29
162	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*, **2018**, 18, 2174-2185	3	29
161	Anti-amyloidogenic and anti-apoptotic effect of □bisabolol against A□induced neurotoxicity in PC12 cells. *European Journal of Medicinal Chemistry*, **2018**, 143, 1196-1207	6.8	28
160	Blocking the interaction between HIV-1 integrase and human LEDGF/p75: mutational studies, virtual screening and molecular dynamics simulations. *Molecular BioSystems*, **2014**, 10, 526-36		28
159	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	3.7	28
158	Exploration of the binding of DNA binding ligands to Staphylococcal DNA through QM/MM docking and molecular dynamics simulation. *Journal of Biomolecular Structure and Dynamics*, **2013**, 31, 561-71	3.6	27
157	In silico screening of indinavir-based compounds targeting proteolytic activity in HIV PR: binding pocket fit approach. *Medicinal Chemistry Research*, **2012**, 21, 4060-4068	2.2	27
156	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, 339-47	5.6	26
155	Identification of potential HIV-1 integrase strand transfer inhibitors: in silico virtual screening and QM/MM docking studies. *SAR and QSAR in Environmental Research*, **2013**, 24, 581-95	3.5	26
154	Shape and pharmacophore-based virtual screening to identify potential cytochrome P450 sterol 14□demethylase inhibitors. *Journal of Receptor and Signal Transduction Research*, **2013**, 33, 234-43	2.6	26
153	Targeting Multidrug Resistant Mycobacterium tuberculosis HtrA2 with Identical Chemical Entities of Fluoroquinolones. *Indian Journal of Pharmaceutical Sciences*, **2012**, 74, 217-22	1.5	26
152	Molecular dynamic simulations reveal suboptimal binding of salbutamol in T164I variant of □2 adrenergic receptor. *PLoS ONE*, **2017**, 12, e0186666	3.7	25
151	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	14	25
150	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	4.2	25
149	Combined ligand and structure-based approaches on HIV-1 integrase strand transfer inhibitors. *Chemico-Biological Interactions*, **2014**, 218, 71-81	5	24
148	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, 1476-83	4	24
147	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, 178-89		23

146	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	3.6	23
145	Molecular docking and structure-based virtual screening studies of potential drug target, CAAX prenyl proteases, of Leishmania donovani. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 2367-86	3.6	22
144	Molecular docking, QPLD, and ADME prediction studies on HIV-1 integrase leads. *Medicinal Chemistry Research*, **2012**, 21, 4239-4251	2.2	22
143	Exploration of fluoroquinolone resistance in Streptococcus pyogenes: comparative structure analysis of wild-type and mutant DNA gyrase. *Journal of Molecular Recognition*, **2013**, 26, 276-85	2.6	22
142	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	1.8	21
141	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	3	21
140	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, 2291-5	1.7	21
139	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, 1686-97	6.1	20
138	E7 oncoprotein of human papillomavirus: Structural dynamics and inhibitor screening study. *Gene*, **2018**, 658, 159-177	3.8	20
137	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	4.5	20
136	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	3.5	20
135	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*, **2018**, 18, 2511-2526	3	20
134	Structural elucidation of SrtA enzyme in Enterococcus faecalis: an emphasis on screening of potential inhibitors against the biofilm formation. *Molecular BioSystems*, **2014**, 10, 1775-89		19
133	Molecular insights on analogs of HIV PR inhibitors toward HTLV-1 PR through QM/MM interactions and molecular dynamics studies: comparative structure analysis of wild and mutant HTLV-1 PR. *Journal of Molecular Recognition*, **2014**, 27, 696-706	2.6	19
132	Biochemical changes in plant leaves as a biomarker of pollution due to anthropogenic activity. *Environmental Monitoring and Assessment*, **2011**, 177, 527-35	3.1	18
131	Identification of Small Molecule as a High Affinity β2 Agonist Promiscuously Targeting Wild and Mutated (Thr164Ile) β 2 Adrenergic Receptor in the Treatment of Bronchial Asthma. *Current Pharmaceutical Design*, **2016**, 22, 5221-5233	3.3	18
130	An In Silico Investigation of Potential EGFR Inhibitors for the Clinical Treatment of Colorectal Cancer. *Current Topics in Medicinal Chemistry*, **2018**, 18, 2355-2366	3	18
129	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	3	18

128	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	1.7	18
127	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	7.9	18
126	Synthesis, antibacterial studies, and molecular modeling studies of 3,4-dihydropyrimidinone compounds. *Journal of Chemical Biology*, **2016**, 9, 31-40		17
125	Comparative structural analysis of two proteins belonging to quorum sensing system in Vibrio cholerae. *Journal of Biomolecular Structure and Dynamics*, **2012**, 30, 574-84	3.6	17
124	Microbe-assisted phytoremediation approach for ecological restoration of zinc mine spoil dump. *International Journal of Environment and Pollution*, **2010**, 43, 236	0.7	17
123	Design of novel JAK3 Inhibitors towards Rheumatoid Arthritis using molecular docking analysis. *Bioinformation*, **2019**, 15, 68-78	1.1	17
122	FLT3 inhibitor design using molecular docking based virtual screening for acute myeloid leukemia. *Bioinformation*, **2019**, 15, 104-115	1.1	17
121	Virtual Screening of IL-6 Inhibitors for Idiopathic Arthritis. *Bioinformation*, **2019**, 15, 121-130	1.1	17
120	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	3.6	17
119	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	2	16
118	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*, **2018**, 18, 2527-2542	3	16
117	Investigating into the molecular interactions of flavonoids targeting NS2B-NS3 protease from ZIKA virus through approaches. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 272-284	3.6	16
116	Design of PD-L1 inhibitors for lung cancer. *Bioinformation*, **2019**, 15, 139-150	1.1	15
115	Dihydroactinidiolide, a natural product against A□nduced toxicity in Neuro2a cells: Synthesis, in silico and in vitro studies. *Bioorganic Chemistry*, **2018**, 81, 340-349	5.1	15
114	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, 1025-40	3.5	14
113	Functional Inhibition of VEGF and EGFR Suppressors in Cancer Treatment. *Current Topics in Medicinal Chemistry*, **2019**, 19, 178-179	3	13
112	Mechanistic Insights into Zika Virus NS3 Helicase Inhibition by Epigallocatechin-3-Gallate. *ACS Omega*, **2020**, 5, 11217-11226	3.9	13
111	Virtual screening based on pharmacophoric features of known calpain inhibitors to identify potent inhibitors of calpain. *Medicinal Chemistry Research*, **2014**, 23, 2445-2455	2.2	13

110	3D-QSAR CoMFA and CoMSIA study on benzodipyrazoles as cyclin dependent kinase 2 inhibitors. *Medicinal Chemistry*, **2008**, 4, 313-21	1.8	13
109	Discovery of Potent Inhibitors for the Inhibition of Dengue Envelope Protein: An In Silico Approach. *Current Topics in Medicinal Chemistry*, **2018**, 18, 1585-1602	3	13
108	Identification of High-affinity Small Molecules Targeting Gamma Secretase for the Treatment of Alzheimer Disease. *Current Topics in Medicinal Chemistry*, **2019**, 19, 1173-1187	3	13
107	Advantages of Structure-Based Drug Design Approaches in Neurological Disorders. *Current Neuropharmacology*, **2017**, 15, 1136-1155	7.6	13
106	Mechanistic insights of SrtA LPXTG blockers targeting the transpeptidase mechanism in Streptococcus mutans. *RSC Advances*, **2015**, 5, 100498-100510	3.7	12
105	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	3.6	12
104	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, 361-71	2.6	12
103	A database for the predicted pharmacophoric features of medicinal compounds. *Bioinformation*, **2011**, 6, 167-8	1.1	12
102	Homology modeling, active site prediction, and targeting the anti hypertension activity through molecular docking on endothelin - B receptor domain. *Bioinformation*, **2012**, 8, 81-6	1.1	12
101	Targeting the cyclin-binding groove site to inhibit the catalytic activity of CDK2/cyclin A complex using p27(KIP1)-derived peptidomimetic inhibitors. *Journal of Chemical Biology*, **2015**, 8, 11-24		11
100	Homology modeling, molecular dynamics, and docking studies of pattern-recognition transmembrane protein-lipopolysaccharide and 1,3 glucan-binding protein from Fenneropenaeus indicus. *Journal of Biomolecular Structure and Dynamics*, **2015**, 33, 1269-80	3.6	11
99	Virtual screening of LPXTG competitive SrtA inhibitors targeting signal transduction mechanism in Bacillus anthracis: a combined experimental and theoretical study. *Journal of Receptor and Signal Transduction Research*, **2014**, 34, 221-32	2.6	11
98	3D-QSAR CoMFA Study on Aminothiazole Derivatives as Cyclin-Dependent Kinase 2 Inhibitors. *QSAR and Combinatorial Science*, **2007**, 26, 85-91		11
97	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	3	11
96	Artificial Intelligence, Big Data and Machine Learning Approaches in Precision Medicine & Drug Discovery. *Current Drug Targets*, **2021**, 22, 631-655	3	11
95	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	3.3	11
94	Cdk5: A main culprit in neurodegeneration. *International Journal of Neuroscience*, **2019**, 129, 1192-1197	2	10
93	Investigations on the interactions of hage-derived peptides against the SrtA mechanism in Bacillus anthracis. *Applied Biochemistry and Biotechnology*, **2014**, 172, 1790-806	3.2	10

92	Investigating the folding pathway and substrate induced conformational changes in B. malayi Guanylate kinase. *International Journal of Biological Macromolecules*, **2017**, 94, 621-633	7.9	10
91	Artificial intelligence and machine learning approaches for drug design: challenges and opportunities for the pharmaceutical industries. *Molecular Diversity*, **2021**, 1	3.1	10
90	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	1.7	10
89	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	3	10
88	An in silico pharmacological approach toward the discovery of potent inhibitors to combat drug resistance HIV-1 protease variants. *Journal of Cellular Biochemistry*, **2019**, 120, 9063-9081	4.7	10
87	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	5	10
86	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	1.8	10
85	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	3.6	9
84	Cyclin Dependent Kinase as Significant Target for Cancer Treatment. *Current Cancer Therapy Reviews*, **2012**, 8, 225-235	0.4	9
83	In Silico Insights on GD2 : A Potential Target for Pediatric Neuroblastoma. *Current Topics in Medicinal Chemistry*, **2019**, 19, 2766-2781	3	9
82	Targeting the NTPase site of Zika virus NS3 helicase for inhibitor discovery. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 4827-4837	3.6	9
81	Comparative analysis of various electrostatic potentials on docking precision against cyclin-dependent kinase 2 protein: a multiple docking approach. *Chemical Biology and Drug Design*, **2015**, 85, 107-18	2.9	8
80	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, 43-9	3	8
79	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	0.6	8
78	E-pharmacophore-based screening of mGluR5 negative allosteric modulators for central nervous system disorder. *Computational Biology and Chemistry*, **2019**, 78, 414-423	3.6	8
77	Interaction investigations of crustacean EGBP recognition toward pathogenic microbial cell membrane and stimulate upon prophenoloxidase activation. *Journal of Molecular Recognition*, **2014**, 27, 173-83	2.6	7
76	In silico Insights on IL-6: A Potential Target for Multicentric Castleman Disease. *Current Computer-Aided Drug Design*, **2020**, 16, 641-653	1.4	7
75	Structure-Based Virtual Screening Reveals Ibrutinib and Zanubrutinib as Potential Repurposed Drugs against COVID-19. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	7

74	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	1.4	7
73	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	2.6	7
72	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, 312-8	3.5	6
71	bisabolol D-fucopyranoside as a potential modulator of amyloid peptide induced neurotoxicity: An in vitro &in silico study. *Bioorganic Chemistry*, **2019**, 88, 102935	5.1	6
70	Daucosterol disturbs redox homeostasis and elicits oxidative-stress mediated apoptosis in A549 cells via targeting thioredoxin reductase by a p53 dependent mechanism. *European Journal of Pharmacology*, **2019**, 855, 112-123	5.3	6
69	Structural dynamic studies on identification of EGCG analogues for the inhibition of Human Papillomavirus E7. *Scientific Reports*, **2020**, 10, 8661	4.9	6
68	Structure based identification and biological evaluation of novel and potent inhibitors of PCAF catalytic domain. *International Journal of Biological Macromolecules*, **2018**, 120, 823-834	7.9	6
67	Ligand-based pharmacophore modelling and screening of DNA minor groove binders targeting Staphylococcus aureus. *Journal of Molecular Recognition*, **2014**, 27, 429-37	2.6	6
66	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	3.6	6
65	An Overview on Zika Virus and the Importance of Computational Drug Discovery. *Journal of Exploratory Research in Pharmacology*, **2018**, 3, 43-51	0.4	6
64	Current Computational Approaches for the Development of Anti-HIV Inhibitors: An Overview. *Current Pharmaceutical Design*, **2019**, 25, 3390-3405	3.3	6
63	Identification of Novel Pancreatic Lipase Inhibitors Using Studies. *Endocrine, Metabolic and Immune Disorders - Drug Targets*, **2019**, 19, 449-457	2.2	6
62	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	1.7	6
61	Modeling of macromolecular proteins in prophenoloxidase cascade through experimental and computational approaches. *Biotechnology and Applied Biochemistry*, **2016**, 63, 779-788	2.8	6
60	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	5.1	5
59	Exploring the Biology and Structural Architecture of Sortase Role on Biofilm Formation in Gram Positive Pathogens. *Current Topics in Medicinal Chemistry*, **2018**, 18, 2462-2480	3	5
58	Functional insights by comparison of modeled structures of 18kDa small heat shock protein and its mutant in Mycobacterium leprae. *Bioinformation*, **2008**, 3, 230-4	1.1	5
57	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	2.2	4

56	Understanding the biological role of PqqB in using molecular dynamics simulation approach. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-13	3.6	4
55	Unravelling novel congeners from acetyllysine mimicking ligand targeting a lysine acetyltransferase PCAF bromodomain. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 4303-4319	3.6	4
54	De Novo Design of Ligands Using Computational Methods. *Methods in Molecular Biology*, **2018**, 1762, 71-86	1.4	4
53	Communication of □phage lysin plyG enzymes binding toward SrtA for inhibition of Bacillus anthracis: protein-protein interaction and molecular dynamics study. *Cell Communication and Adhesion*, **2014**, 21, 257-65		4
52	Explicit Drug Re-positioning: Predicting Novel Drug-Target Interactions of the Shelved Molecules with QM/MM Based Approaches. *Advances in Protein Chemistry and Structural Biology*, **2015**, 100, 89-112	5.3	4
51	Exploration of protein-protein interaction effects on □2-macroglobulin in an inhibition of serine protease through gene expression and molecular simulations studies. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 1841-54	3.6	4
50	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	1.3	4
49	strategies for identification of potent inhibitor for MMP-1 to prevent metastasis of breast cancer. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 7274-7293	3.6	4
48	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, 186-98	2.6	4
47	Competitive Inhibition of Quercetin and Apigenin at the ATP Binding site of D-Alanine-D-Alanine Ligase of Helicobacter pylori □A Molecular Modeling Approach. *Current Biotechnology*, **2019**, 7, 340-348	0.6	4
46	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	1.5	4
45	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	3.6	4
44	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	2	4
43	Natural vs. reclaimed forests □a case study of successional change, reclamation technique and phytodiversity. *International Journal of Mining, Reclamation and Environment*, **2015**, 29, 476-498	2.2	3
42	Understanding the importance of conservative hypothetical protein LdBPK_070020 in Leishmania donovani and its role in subsistence of the parasite. *Archives of Biochemistry and Biophysics*, **2016**, 596, 10-21	4.1	3
41	Deciphering the binding mode and mechanistic insights of pentadecylidenemalonate (1b) as activator of histone acetyltransferase PCAF. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 2296-2309	3.6	3
40	Pharmacophoric features of nucleosidic HIV-1RT inhibitors. *Bioorganic and Medicinal Chemistry*, **2003**, 11, 1801-7	3.4	3
39	Common binding mode for structurally and chemically diverse non-nucleosidic HIV-1RT inhibitors. *Computational and Theoretical Chemistry*, **2005**, 723, 205-209		3

38	Identification of Potential Dual Negative Allosteric Modulators of Group I mGluR Family: A Shape Based Screening, ADME Prediction, Induced Fit Docking and Molecular Dynamics Approach Against Neurodegenerative Diseases. *Current Topics in Medicinal Chemistry*, **2019**, 19, 2687-2707	3	3
37	Mechanistic insights into Zika virus NS3 helicase inhibition by Epigallocatechin-3-gallate		3
36	Computational identification and antifungal bioassay reveals phytosterols as potential inhibitor of. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 1143-1157	3.6	3
35	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	5.3	3
34	Interrogation of 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	4	3
33	Structural Understanding of SARS-CoV-2 Drug Targets, Active Site Contour Map Analysis and COVID-19 Therapeutics. *Current Molecular Pharmacology*, **2021**,	3.7	3
32	Molecular cloning, relative expression, and structural analysis of pattern recognition molecule Eglucan binding protein from mangrove crab Episesarma tetragonum. *Biotechnology and Applied Biochemistry*, **2015**, 62, 416-23	2.8	2
31	Computational analysis identifies druggable mutations in human rBAT mediated Cystinuria. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 5058-5067	3.6	2
30	A replica placement and replacement algorithm for data-grid in DRTDBS **2014**,		2
29	An ab initio quantum mechanical drug designing procedure: application to the design of balanced dual ACE/NEP inhibitors. *Journal of Molecular Modeling*, **2009**, 15, 1447-62	2	2
28	Phage Protein Interactions in the Inhibition Mechanism of Bacterial Cell **2020**, 121-142		2
27	Homology modeling and in silico site directed mutagenesis of pyruvate ferredoxin oxidoreductase from Clostridium thermocellum. *Combinatorial Chemistry and High Throughput Screening*, **2015**, 18, 975-89	1.3	2
26	Ion Channels as Therapeutic Targets for Type 1 Diabetes Mellitus. *Current Drug Targets*, **2020**, 21, 132-147	3	2
25	Effect of HIV-1 Subtype C integrase mutations implied using molecular modeling and docking data. *Bioinformation*, **2016**, 12, 221-230	1.1	2
24	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	3.7	2
23	Effect of Amino Acid Substitution in the Penaeus monodon LGBP and Specificity Through Mutational Analysis. *International Journal of Peptide Research and Therapeutics*, **2020**, 26, 1789-1801	2.1	2
22	Experiments and simulation on ZIKV NS2B-NS3 protease reveal its complex folding. *Virology*, **2021**, 556, 110-123	3.6	2
21	Identification and Characterization of Lipopeptide Biosurfactant Producing sp Isolated from Brackish River Water. *Current Topics in Medicinal Chemistry*, **2020**, 20, 2221-2234	3	1

20	Carbon Sequestration in Terrestrial Ecosystems. *Environmental Chemistry for A Sustainable World*, **2015**, 99-131	0.8	1
19	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	3.9	1
18	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	7.9	1
17	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	3.6	1
16	Subcellular localization studies of LdBPK_070020, a conserved protein of. *Journal of Vector Borne Diseases*, **2016**, 53, 375-378	0.7	1
15	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*,1-21	2	1
14	Drug discovery for cancer therapy with special reference to inhibitors of protein kinase pathway **2022**, 71-96		1
13	Fragment-Based De Novo Design of Cyclin-Dependent Kinase 2 Inhibitors. *Methods in Molecular Biology*, **2016**, 1336, 47-58	1.4	0
12	Immunological insights of selectins in human disease mechanism.. *Advances in Protein Chemistry and Structural Biology*, **2022**, 129, 163-188	5.3	0
11	Chemoinformatics and QSAR **2021**, 183-212		0
10	Characterization and structural analysis of prophenoloxidase in mud crab Scylla serrata and discovering novel chemical inhibitors through virtual screening. *Structural Chemistry*, **2020**, 31, 1563-1584	1.8	
9	Protein-Protein Interaction for the De Novo Design of Cyclin-Dependent Kinase Peptide Inhibitors. *Methods in Molecular Biology*, **2016**, 1336, 59-66	1.4	
8	Threshold interaction energy of NRTIQ (2Qdeoxy 3Qsubstituted nucleosidic analogs of reverse transcriptase inhibitors) to undergo competitive inhibition. *Bioorganic and Medicinal Chemistry Letters*, **2004**, 14, 2677-80	2.9	
7	Envisaging the conformational space of proteins by coupling machine learning and molecular dynamics **2022**, 467-475		
6	Molecular interaction analysis of 1, 3 glucan binding protein with Bacillus licheniformis and evaluation of its immunostimulant property in Oreochromis mossambicus.. *Fish and Shellfish Immunology*, **2021**, 121, 183-183	4.3	
5	Predicting Protein Folding and Protein Stability by Molecular Dynamics Simulations for Computational Drug Discovery **2021**, 153-177		
4	Omics-Based Nanomedicine **2018**, 227-248		
3	Medicinal Application of Synthetic Biology **2018**, 87-94		

2	Magnitude and Advancements of CADD in Identifying Therapeutic Intervention against Flaviviruses **2021**, 179-203	
1	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	5.3