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	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
3	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
4	Molecular interaction analysis of Î²-1, 3 glucan binding protein with Bacillus licheniformis and evaluation of its immunostimulant property in Oreochromis mossambicus. Fish and Shellfish Immunology, 2022, 121, 183-196.	1.6	2
5	Envisaging the conformational space of proteins by coupling machine learning and molecular dynamics. , 2022, , 467-475.		0
6	Immunological insights of selectins in human disease mechanism. Advances in Protein Chemistry and Structural Biology, 2022, 129, 163-188.	1.0	2
7	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
8	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
9	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
10	Drug discovery for cancer therapy with special reference to inhibitors of protein kinase pathway. , 2022, , 71-96.		2
11	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
12	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
13	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
14	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
15	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
16	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
17	Predicting Protein Folding and Protein Stability by Molecular Dynamics Simulations for Computational Drug Discovery. , 2021, , 153-177.		0
18	Chemoinformatics and QSAR. , 2021, , 183-212.		1

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19	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
20	Experiments and simulation on ZIKV NS2B-NS3 protease reveal its complex folding. Virology, 2021, 556, 110-123.	1.1	4
21	Artificial Intelligence, Big Data and Machine Learning Approaches in Precision Medicine & Drug Discovery. Current Drug Targets, 2021, 22, 631-655.	1.0	32
22	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
23	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
24	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
25	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
26	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
27	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
28	Structural Understanding of SARS-CoV-2 Drug Targets, Active Site Contour Map Analysis and COVID-19 Therapeutics. Current Molecular Pharmacology, 2021, 14, .	0.7	4
29	Magnitude and Advancements of CADD in Identifying Therapeutic Intervention against Flaviviruses. , 2021, , 179-203.		2
30	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
31	A Review on Pharmacokinetics Properties of Antiretroviral Drugs to Treat HIV-1 Infections. Current Computer-Aided Drug Design, 2021, 17, 850-864.	0.8	3
32	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
33	Computational identification and antifungal bioassay reveals phytosterols as potential inhibitor of Alternaria arborescens. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1143-1157.	2.0	4
34	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
35	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
36	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

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37	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
38	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.	0.9	2
39	Constitutive Inflammatory Cytokine Storm: A Major Threat to Human Health. Journal of Interferon and Cytokine Research, 2020, 40, 19-23.	0.5	78
40	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
41	Mechanistic Insights into Zika Virus NS3 Helicase Inhibition by Epigallocatechin-3-Gallate. ACS Omega, 2020, 5, 11217-11226.	1.6	25
42	Structural dynamic studies on identification of EGCG analogues for the inhibition of Human Papillomavirus E7. Scientific Reports, 2020, 10, 8661.	1.6	15
43	Computational analysis identifies druggable mutations in human rBAT mediated Cystinuria. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-10.	2.0	2
44	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
45	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.	1.0	1
46	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
47	Ion Channels as Therapeutic Targets for Type 1 Diabetes Mellitus. Current Drug Targets, 2020, 21, 132-147.	1.0	7
48	In Silico Insights on GD2 : A Potential Target for Pediatric Neuroblastoma. Current Topics in Medicinal Chemistry, 2020, 19, 2766-2781.	1.0	14
49	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
50	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
51	Phage Protein Interactions in the Inhibition Mechanism of Bacterial Cell. , 2020, , 121-142.		2
52	Identification and Characterization of Lipopeptide Biosurfactant Producing Microbacterium sp Isolated from Brackish River Water. Current Topics in Medicinal Chemistry, 2020, 20, 2221-2234.	1.0	3
53	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.	2.0	3
54	Cdk5: A main culprit in neurodegeneration. International Journal of Neuroscience, 2019, 129, 1192-1197.	0.8	17

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55	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
56	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
57	Functional Inhibition of VEGF and EGFR Suppressors in Cancer Treatment. Current Topics in Medicinal Chemistry, 2019, 19, 178-179.	1.0	18
58	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
59	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
60	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
61	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
62	Current Computational Approaches for the Development of Anti-HIV Inhibitors: An Overview. Current Pharmaceutical Design, 2019, 25, 3390-3405.	0.9	13
63	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
64	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
65	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
66	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
67	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
68	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
69	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
70	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.	1.0	3
71	Identification of Novel Pancreatic Lipase Inhibitors UsingIn SilicoStudies. Endocrine, Metabolic and Immune Disorders - Drug Targets, 2019, 19, 449-457.	0.6	12
72	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

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73	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
74	Design of novel JAK3 Inhibitors towards Rheumatoid Arthritis using molecular docking analysis. Bioinformation, 2019, 15, 68-78.	0.2	27
75	FLT3 inhibitor design using molecular docking based virtual screening for acute myeloid leukemia. Bioinformation, 2019, 15, 104-115.	0.2	24
76	Virtual Screening of IL-6 Inhibitors for Idiopathic Arthritis. Bioinformation, 2019, 15, 121-130.	0.2	24
77	Design of PD-L1 inhibitors for lung cancer. Bioinformation, 2019, 15, 139-150.	0.2	25
78	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
79	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
80	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
81	De Novo Design of Ligands Using Computational Methods. Methods in Molecular Biology, 2018, 1762, 71-86.	0.4	8
82	E7 oncoprotein of human papillomavirus: Structural dynamics and inhibitor screening study. Gene, 2018, 658, 159-177.	1.0	30
83	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
84	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
85	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
86	Anti-amyloidogenic and anti-apoptotic effect of Î±-bisabolol against AÎ²2 induced neurotoxicity in PC12 cells. European Journal of Medicinal Chemistry, 2018, 143, 1196-1207.	2.6	37
87	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
88	Screening, isolation and characterization of biosurfactant producing Bacillus subtilis strain ANSKLAB03. Bioinformation, 2018, 14, 304-314.	0.2	71
89	Hydroxychloroquine Inhibits Zika Virus NS2B-NS3 Protease. ACS Omega, 2018, 3, 18132-18141.	1.6	86
90	Omics-Based Nanomedicine. , 2018, , 227-248.		0

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91	Medicinal Application of Synthetic Biology. , 2018, , 87-94.		0
92	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
93	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
94	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
95	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
96	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
97	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
98	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
99	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
100	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
101	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
102	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
103	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
104	Molecular dynamic simulations reveal suboptimal binding of salbutamol in T164I variant of Î²2 adrenergic receptor. PLoS ONE, 2017, 12, e0186666.	1.1	34
105	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
106	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
107	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
108	Advantages of Structure-Based Drug Design Approaches in Neurological Disorders. Current Neuropharmacology, 2017, 15, 1136-1155.	1.4	23

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109	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
110	Modeling of macromolecular proteins in prophenoloxidase cascade through experimental and computational approaches. Biotechnology and Applied Biochemistry, 2016, 63, 779-788.	1.4	7
111	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
112	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
113	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.	1.4	4
114	Protein-Protein Interaction for the De Novo Design of Cyclin-Dependent Kinase Peptide Inhibitors. Methods in Molecular Biology, 2016, 1336, 59-66.	0.4	1
115	Fragment-Based De Novo Design of Cyclin-Dependent Kinase 2 Inhibitors. Methods in Molecular Biology, 2016, 1336, 47-58.	0.4	2
116	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
117	Synthesis, antibacterial studies, and molecular modeling studies of 3,4-dihydropyrimidinone compounds. Journal of Chemical Biology, 2016, 9, 31-40.	2.2	26
118	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
119	Effect of HIV-1 Subtype C integrase mutations implied using molecular modeling and docking data. Bioinformation, 2016, 12, 221-230.	0.2	5
120	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
121	Subcellular localization studies of LdBPK_070020, a conserved protein of. Journal of Vector Borne Diseases, 2016, 53, 375-378.	0.1	1
122	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
123	Explicit Drug Re-positioning. Advances in Protein Chemistry and Structural Biology, 2015, 100, 89-112.	1.0	4
124	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
125	Molecular cloning, relative expression, and structural analysis of pattern recognition molecule Î²â€glucan binding protein from mangrove crab Episesarma tetragonum. Biotechnology and Applied Biochemistry, 2015, 62, 416-423.	1.4	2
126	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

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127	Frontal facial images based age classify via SVM. , 2015, , .		1
128	Dynamic load balancing using buffer management in distributed database environment. , 2015, , .		2
129	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
130	Mechanistic insights of SrtAâ€“LPXTG blockers targeting the transpeptidase mechanism in Streptococcus mutans. RSC Advances, 2015, 5, 100498-100510.	1.7	15
131	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
132	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
133	Comparative Analysis of Various Electrostatic Potentials on Docking Precision Against Cyclinâ€Dependent Kinase 2 Protein: A Multiple Docking Approach. Chemical Biology and Drug Design, 2015, 85, 107-118.	1.5	9
134	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
135	Carbon Sequestration in Terrestrial Ecosystems. Environmental Chemistry for A Sustainable World, 2015, , 99-131.	0.3	3
136	Homology modeling and in silico site directed mutagenesis of pyruvate ferredoxin oxidoreductase from Clostridium thermocellum. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 975-989.	0.6	2
137	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
138	A replica placement and replacement algorithm for data-grid in DRTDBS. , 2014, , .		2
139	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
140	Application of artificial immune system approach to develop an algorithm for optimizing multi objective problems. , 2014, , .		0
141	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
142	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
143	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
144	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

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145	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
146	Combined ligand and structure-based approaches on HIV-1 integrase strand transfer inhibitors. Chemico-Biological Interactions, 2014, 218, 71-81.	1.7	29
147	Ligand-based pharmacophore modelling and screening of DNA minor groove binders targetingStaphylococcus aureus. Journal of Molecular Recognition, 2014, 27, 429-437.	1.1	6
148	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
149	Image processing capabilities in distributed real time database systems. , 2014, , .		1
150	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
151	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
152	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
153	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
154	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
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