Chiragkumar N Patel

List of Publications by Year
in descending order

50	900	516215 16	552369 26
papers	citations	h-index	g-index

56	56	56	1101
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Excavating phytochemicals from plants possessing antiviral activities for identifying SARS-CoV hemagglutinin-esterase inhibitors by diligent computational workflow. Journal of Biomolecular Structure and Dynamics, 2023, 41, 2382-2397.	2.0	5
2	Molecular docking studies of phytocompounds ofRheum emodiWall with proteins responsible for antibiotic resistance in bacterial and fungal pathogens:in silicoapproach to enhance the bio-availability of antibiotics. Journal of Biomolecular Structure and Dynamics, 2022, 40, 3789-3803.	2.0	24
3	Repurposing of anticancer phytochemicals for identifying potential fusion inhibitor for SARS-CoV-2 using molecular docking and molecular dynamics (MD) simulations. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7744-7761.	2.0	16
4	In vitroandin silicoanalysisof Thymus serpyllumessential oil as bioactivity enhancer of antibacterial and antifungal agents. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10383-10402.	2.0	20
5	Antihypertensive activity of phytocompounds from selected medicinal plants via inhibition of angiotensin-converting enzyme (ACE) protein: an in-silico approach. Natural Product Research, 2022, 36, 4526-4529.	1.0	5
6	In vitroandin silicoantioxidant and anti-inflammatory potential of essential oil ofCymbopogon citratus(DC.) Stapf. of North-Western Himalaya. Journal of Biomolecular Structure and Dynamics, 2022, 40, 14131-14145.	2.0	10
7	Calix[4]pyrrole based scrupulous probe for track on of tryptophan: Host-guest interaction, in silico modeling and molecular docking insights. Chemical Physics, 2022, 554, 111426.	0.9	9
8	Theaflavin-3-gallate, a natural antagonist for Hsp90: In-silico and in-vitro approach. Chemico-Biological Interactions, 2022, 353, 109774.	1.7	5
9	<scp>PharmRF</scp>: A machineâ€learning scoring function to identify the best proteinâ€ligand complexes for structureâ€based pharmacophore screening with high enrichments. Journal of Computational Chemistry, 2022, 43, 847-863.	1.5	2
10	Methylxanthines as Potential Inhibitor of SARS-CoV-2: an In Silico Approach. Current Pharmacology Reports, 2022, 8, 149-170.	1.5	15
11	Novel edifice calix[4]pyrrole derivatives as a potential sensor for the detection of analytes and in silico computational behaviour. Talanta Open, 2022, 5, 100115.	1.7	3
12	Metabolic Profile, Biotransformation, Docking Studies and Molecular Dynamics Simulations of Bioactive Compounds Secreted by CG3 Strain. Antibiotics, 2022, 11, 657.	1.5	3
13	A new N-methylhydrazinecarbothioamide incorporated â€œnaked-eyeâ€•and â€œturn-offâ€•chemosensor for selective and low detection of Cu2+ ions and computation study. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 408, 113097.	2.0	20
14	Identification of potential inhibitors of coronavirus hemagglutinin-esterase using molecular docking, molecular dynamics simulation and binding free energy calculation. Molecular Diversity, 2021, 25, 421-433.	2.1	26
15	In-Silico analysis reveals lower transcription efficiency of C241T variant of SARS-CoV-2 with host replication factors MADP1 and hnRNP-1. Informatics in Medicine Unlocked, 2021, 25, 100670.	1.9	16
16	Berries anthocyanins as potential SARS-CoVâ€“2 inhibitors targeting the viral attachment and replication; molecular docking simulation. Egyptian Journal of Petroleum, 2021, 30, 33-43.	1.2	23
17	Pinpointing the potential hits for hindering interaction of SARS-CoV-2 S-protein with ACE2 from the pool of antiviral phytochemicals utilizing molecular docking and molecular dynamics (MD) simulations. Journal of Molecular Graphics and Modelling, 2021, 105, 107874.	1.3	37
18	Identification of novel inhibitors of <scp>SARSâ€CoV</scp>â€2 main protease (M^{pro}) from Withania sp. by molecular docking and molecular dynamics simulation. Journal of Computational Chemistry, 2021, 42, 1861-1872.	1.5	21

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19	Identification of antiviral phytochemicals as a potential SARS-CoV-2 main protease (Mpro) inhibitor using docking and molecular dynamics simulations. Scientific Reports, 2021, 11, 20295.	1.6	24
20	A multiparametric organ toxicity predictor for drug discovery. Toxicology Mechanisms and Methods, 2020, 30, 159-166.	1.3	16
21	In silico and inÂvitro studies to elucidate the role of 1HYN and 1QKI activity in BPA induced toxicity and its amelioration by Gallic acid. Chemosphere, 2020, 241, 125076.	4.2	7
22	Novel isoniazid-spirooxindole derivatives: design, synthesis, biological evaluation, in silico ADMET prediction and computational studies. Journal of Molecular Structure, 2020, 1222, 128881.	1.8	13
23	Development of cardiotoxicity model using ligand-centric and receptor-centric descriptors. Toxicology Research and Application, 2020, 4, 239784732097125.	0.7	0
24	Identification of promising compounds from curry tree with cyclooxygenase inhibitory potential using a combination of machine learning, molecular docking, dynamics simulations and binding free energy calculations. Molecular Simulation, 2020, 46, 812-822.	0.9	9
25	In silico prediction of potential inhibitors for the main protease of SARS-CoV-2 using molecular docking and dynamics simulation based drug-repurposing. Journal of Infection and Public Health, 2020, 13, 1210-1223.	1.9	203
26	Structural motifs of oxacalix[4]arene for molecular recognition of nitroaromatic explosives: Experimental and computational investigations of host-guest complexes. Journal of Molecular Liquids, 2020, 306, 112809.	2.3	21
27	Synthesis and computational mechanistic studies of copper selective molecular receptor. Vietnam Journal of Chemistry, 2020, 58, 221-230.	0.7	5
28	Energetic contributions of amino acid residues and its crossâ€talk to delineate ligandâ€binding mechanism. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1207-1225.	1.5	16
29	Cardiotonic steroids as potential Na⁺/K⁺-ATPase inhibitors â€“ a computational study. Journal of Receptor and Signal Transduction Research, 2019, 39, 226-234.	1.3	15
30	Calix[4]pyrrole virtuous sensor: a selective and sensitive recognition for Pb(II) ions by spectroscopic and computational study. Supramolecular Chemistry, 2019, 31, 268-282.	1.5	11
31	Synthesis, biological evaluation and computational study of novel isoniazid containing 4H-Pyrimido[2,1-b]benzothiazoles derivatives. European Journal of Medicinal Chemistry, 2019, 177, 12-31.	2.6	20
32	Facile construction & modeling of a highly active thiacalixphenyl[4]arene-protected nano-palladium catalyst for various Câ€“C cross-coupling reactions. New Journal of Chemistry, 2019, 43, 5611-5622.	1.4	3
33	Pharmacophore-based virtual screening of catechol-o-methyltransferase (COMT) inhibitors to combat Alzheimerâ€™s disease. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3938-3957.	2.0	51
34	Dual in vitro and in silico analysis of thiacalix[4]arene dinaphthalene sulfonate for the sensing of 4-nitrotoluene and 2,3-dinitrotoluene. New Journal of Chemistry, 2018, 42, 2682-2691.	1.4	19
35	Microwave-Assisted ZrSiO2 Catalysed Synthesis, Characterization and Computational Study of Novel Spiro[Indole-Thiazolidines] Derivatives as Anti-tubercular Agents. Interdisciplinary Sciences, Computational Life Sciences, 2018, 10, 411-418.	2.2	15
36	The effect of bisphenol A on testicular steroidogenesis and its amelioration by quercetin: anin vivoandin silicoapproach. Toxicology Research, 2018, 7, 22-31.	0.9	18

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37	Facile Construction and In Silico Study of Quinolineâ€Attached Resorcinarene Fluorescent Sensor for the Recognition of Insensitive Munition Compounds. ChemistrySelect, 2018, 3, 12951-12959.	0.7	5
38	Targeting epidermal growth factor receptors inhibition in non-small-cell lung cancer: a computational approach. Molecular Simulation, 2018, 44, 1478-1488.	0.9	10
39	receptor and its spectral analysis. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 204, 581-589.	2.0	13
40	Ameliorative effects of quercetin against bisphenol A-caused oxidative stress in human erythrocytes: anin vitroandin silico study. Toxicology Research, 2018, 7, 1091-1099.	0.9	23
41	Design and synthesis of two armed molecular receptor for recognition of Gd³⁺ metal ion and its computational study. Applied Organometallic Chemistry, 2018, 32, e4502.	1.7	13
42	Parallel screening of drug-like natural compounds using Caco-2 cell permeability QSAR model with applicability domain, lipophilic ligand efficiency index and shape property: A case study of HIV-1 reverse transcriptase inhibitors. Journal of Molecular Structure, 2017, 1146, 80-95.	1.8	13
43	Molecular dynamics-assisted pharmacophore modeling of caspase-3-isatin sulfonamide complex: Recognizing essential intermolecular contacts and features of sulfonamide inhibitor class for caspase-3 binding. Computational Biology and Chemistry, 2017, 71, 117-128.	1.1	11
44	Highly selective and sensitive fluorescent sensor: Thiacalix[4]arene-1-naphthalene carboxylate for Zn2+ ions. Journal of Molecular Structure, 2017, 1133, 1-8.	1.8	21
45	A resorcinarene-based â€œturn-offâ€•fluorescence sensor for 4-nitrotoluene: Insights from fluorescence and 1 H NMR titration with computational approach. Journal of Luminescence, 2017, 184, 74-82.	1.5	26
46	Retrieval of promiscuous natural compounds using multiple targets docking strategy: A case study on kinase polypharmacology. , 2017, , .		2
47	Antiproliferative Efficacy of Kaempferol on Cultured Daudi Cells: An In Silico and In Vitro Study. Advances in Biology, 2016, 2016, 1-10.	1.2	6
48	Thiacalix[4]arene-tetra-(quinoline-8- sulfonate): a Sensitive and Selective Fluorescent Sensor for Co (II). Journal of Fluorescence, 2016, 26, 1729-1736.	1.3	21
49	Regression Correlation Analysis between GBH and Carbon Stock of Major Tree Species in Dharoi Range, Gandhinagar Forest Division, India. International Journal of Innovative Research in Science, Engineering and Technology, 2014, 03, 17146-17149.	0.4	1
50	Analyzing the role of phytochemicals in targeting drug transporter protein ABCC6 using molecular docking and molecular dynamics simulations. International Journal of Pharmaceutical Sciences and Drug Research, 0, , 275-281.	0.1	4