

Chiragkumar N Patel

List of Publications by Year in descending order

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50
papers

900
citations

516215

16
h-index

552369

26
g-index

56
all docs

56
docs citations

56
times ranked

1101
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	Pharmacophore-based virtual screening of catechol-o-methyltransferase (COMT) inhibitors to combat Alzheimer's disease. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3938-3957.	2.0	51
3	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
4	A resorcinarene-based "turn-off" 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
5	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
6	Molecular docking studies of phytochemicals of <i>Rheum emodi</i> Wall with proteins responsible for antibiotic resistance in bacterial and fungal pathogens: <i>in silico</i> approach to enhance the bio-availability of antibiotics. Journal of Biomolecular Structure and Dynamics, 2022, 40, 3789-3803.	2.0	24
7	Identification of antiviral phytochemicals as a potential SARS-CoV-2 main protease (M ^{pro}) inhibitor using docking and molecular dynamics simulations. Scientific Reports, 2021, 11, 20295.	1.6	24
8	Ameliorative effects of quercetin against bisphenol A-caused oxidative stress in human erythrocytes: an <i>in vitro</i> and <i>in silico</i> study. Toxicology Research, 2018, 7, 1091-1099.	0.9	23
9	Berries anthocyanins as potential SARS-CoV-2 inhibitors targeting the viral attachment and replication; molecular docking simulation. Egyptian Journal of Petroleum, 2021, 30, 33-43.	1.2	23
10	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
11	Highly selective and sensitive fluorescent sensor: Thiacalix[4]arene-1-naphthalene carboxylate for Zn ²⁺ ions. Journal of Molecular Structure, 2017, 1133, 1-8.	1.8	21
12	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
13	Identification of novel inhibitors of SARS-CoV-2 main protease (M ^{pro}) from <i>Withania</i> sp. by molecular docking and molecular dynamics simulation. Journal of Computational Chemistry, 2021, 42, 1861-1872.	1.5	21
14	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
15	A new N-methylhydrazinecarbothioamide incorporated "naked-eye" and "turn-off" chemosensor for selective and low detection of Cu ²⁺ ions and computation study. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 408, 113097.	2.0	20
16	<i>In vitro</i> and <i>in silico</i> analysis of Thymus serpyllum essential oil as bioactivity enhancer of antibacterial and antifungal agents. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10383-10402.	2.0	20
17	Dual <i>in vitro</i> and <i>in silico</i> 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
18	The effect of bisphenol A on testicular steroidogenesis and its amelioration by quercetin: an <i>in vivo</i> and <i>in silico</i> approach. Toxicology Research, 2018, 7, 22-31.	0.9	18

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19	A multiparametric organ toxicity predictor for drug discovery. <i>Toxicology Mechanisms and Methods</i> , 2020, 30, 159-166.	1.3	16
20	Energetic contributions of amino acid residues and its cross-talk to delineate ligand-binding mechanism. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020, 88, 1207-1225.	1.5	16
21	In-Silico analysis reveals lower transcription efficiency of C241T variant of SARS-CoV-2 with host replication factors MADP1 and hnRNP-1. <i>Informatics in Medicine Unlocked</i> , 2021, 25, 100670.	1.9	16
22	Repurposing of anticancer phytochemicals for identifying potential fusion inhibitor for SARS-CoV-2 using molecular docking and molecular dynamics (MD) simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 7744-7761.	2.0	16
23	Microwave-Assisted ZrSiO ₂ Catalysed Synthesis, Characterization and Computational Study of Novel Spiro[Indole-Thiazolidines] Derivatives as Anti-tubercular Agents. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2018, 10, 411-418.	2.2	15
24	Cardiotonic steroids as potential Na ⁺ /K ⁺ -ATPase inhibitors – a computational study. <i>Journal of Receptor and Signal Transduction Research</i> , 2019, 39, 226-234.	1.3	15
25	Methylxanthines as Potential Inhibitor of SARS-CoV-2: an In Silico Approach. <i>Current Pharmacology Reports</i> , 2022, 8, 149-170.	1.5	15
26	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. <i>Journal of Molecular Structure</i> , 2017, 1146, 80-95.	1.8	13
27	receptor and its spectral analysis. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 204, 581-589.	2.0	13
28	Design and synthesis of two armed molecular receptor for recognition of Gd ³⁺ metal ion and its computational study. <i>Applied Organometallic Chemistry</i> , 2018, 32, e4502.	1.7	13
29	Novel isoniazid-spirooxindole derivatives: design, synthesis, biological evaluation, in silico ADMET prediction and computational studies. <i>Journal of Molecular Structure</i> , 2020, 1222, 128881.	1.8	13
30	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. <i>Computational Biology and Chemistry</i> , 2017, 71, 117-128.	1.1	11
31	Calix[4]pyrrole virtuous sensor: a selective and sensitive recognition for Pb(II) ions by spectroscopic and computational study. <i>Supramolecular Chemistry</i> , 2019, 31, 268-282.	1.5	11
32	Targeting epidermal growth factor receptors inhibition in non-small-cell lung cancer: a computational approach. <i>Molecular Simulation</i> , 2018, 44, 1478-1488.	0.9	10
33	<i>In vitro</i> and <i>in silico</i> antioxidant and anti-inflammatory potential of essential oil of <i>Cymbopogon citratus</i> (DC.) Stapf. of North-Western Himalaya. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 14131-14145.	2.0	10
34	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. <i>Molecular Simulation</i> , 2020, 46, 812-822.	0.9	9
35	Calix[4]pyrrole based scrupulous probe for track on of tryptophan: Host-guest interaction, in silico modeling and molecular docking insights. <i>Chemical Physics</i> , 2022, 554, 111426.	0.9	9
36	In silico and <i>in vitro</i> studies to elucidate the role of 1HYN and 1QKI activity in BPA induced toxicity and its amelioration by Gallic acid. <i>Chemosphere</i> , 2020, 241, 125076.	4.2	7

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37	Antiproliferative Efficacy of Kaempferol on Cultured Daudi Cells: An <i>In Silico</i> and <i>In Vitro</i> Study. <i>Advances in Biology</i> , 2016, 2016, 1-10.	1.2	6
38	Facile Construction and <i>In Silico</i> Study of Quinoline-Attached Resorcinarene Fluorescent Sensor for the Recognition of Insensitive Munition Compounds. <i>ChemistrySelect</i> , 2018, 3, 12951-12959.	0.7	5
39	Synthesis and computational mechanistic studies of copper selective molecular receptor. <i>Vietnam Journal of Chemistry</i> , 2020, 58, 221-230.	0.7	5
40	Antihypertensive activity of phytochemicals from selected medicinal plants via inhibition of angiotensin-converting enzyme (ACE) protein: an <i>in-silico</i> approach. <i>Natural Product Research</i> , 2022, 36, 4526-4529.	1.0	5
41	Excavating phytochemicals from plants possessing antiviral activities for identifying SARS-CoV hemagglutinin-esterase inhibitors by diligent computational workflow. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 2382-2397.	2.0	5
42	Theaflavin-3-gallate, a natural antagonist for Hsp90: <i>In-silico</i> and <i>in-vitro</i> approach. <i>Chemico-Biological Interactions</i> , 2022, 353, 109774.	1.7	5
43	Analyzing the role of phytochemicals in targeting drug transporter protein ABCC6 using molecular docking and molecular dynamics simulations. <i>International Journal of Pharmaceutical Sciences and Drug Research</i> , 0, , 275-281.	0.1	4
44	Facile construction & modeling of a highly active thiacalixphenyl[4]arene-protected nano-palladium catalyst for various C-C cross-coupling reactions. <i>New Journal of Chemistry</i> , 2019, 43, 5611-5622.	1.4	3
45	Novel edifice calix[4]pyrrole derivatives as a potential sensor for the detection of analytes and <i>in silico</i> computational behaviour. <i>Talanta Open</i> , 2022, 5, 100115.	1.7	3
46	Metabolic Profile, Biotransformation, Docking Studies and Molecular Dynamics Simulations of Bioactive Compounds Secreted by CG3 Strain. <i>Antibiotics</i> , 2022, 11, 657.	1.5	3
47	Retrieval of promiscuous natural compounds using multiple targets docking strategy: A case study on kinase polypharmacology. , 2017, , .		2
48	PharmRF: A machine-learning scoring function to identify the best protein-ligand complexes for structure-based pharmacophore screening with high enrichments. <i>Journal of Computational Chemistry</i> , 2022, 43, 847-863.	1.5	2
49	Regression Correlation Analysis between GBH and Carbon Stock of Major Tree Species in Dharoi Range, Gandhinagar Forest Division, India. <i>International Journal of Innovative Research in Science, Engineering and Technology</i> , 2014, 03, 17146-17149.	0.4	1
50	Development of cardiotoxicity model using ligand-centric and receptor-centric descriptors. <i>Toxicology Research and Application</i> , 2020, 4, 239784732097125.	0.7	0