Deepak K Lokwani

List of Publications by Year
in descending order

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46 papers	763 citations	430874 18 h-index	580821 25 g-index
46 all docs	46 docs citations	46 times ranked	965 citing authors

#	Article	IF	Citations
1	In silico screening of phytopolyphenolics for the identification of bioactive compounds as novel protease inhibitors effective against SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10437-10453.	3.5	49
2	Structure Based Library Design (SBLD) for new 1,4-dihydropyrimidine scaffold as simultaneous COX-1/COX-2 and 5-LOX inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 4533-4543.	3.0	42
3	A new efficient domino approach for the synthesis of coumarin-pyrazolines as antimicrobial agents targeting bacterial<scp>d</scp>-alanine-<scp>d</scp>-alanine ligase. New Journal of Chemistry, 2019, 43, 9002-9011.	2.8	36
4	Ultrasound Mediated One-Pot, Three Component Synthesis, Docking and ADME Prediction of Novel 5-Amino-2-(4-chlorophenyl)-7-Substituted Phenyl-8,8a-dihydro-7H-(1,3,4)thiadiazolo(3,2-Î±)pyrimidine-6-carbonitrile Derivatives as Anticancer Agents. Molecules, 2016, 21, 894.	3.8	35
5	DIPEAc promoted one-pot synthesis of dihydropyrido[2,3-d:6,5-dâ€²]dipyrimidinetetraone and pyrimido[4,5-d]pyrimidine derivatives as potent tyrosinase inhibitors and anticancer agents: in vitro screening, molecular docking and ADMET predictions. New Journal of Chemistry, 2018, 42, 18621-18632.	2.8	34
6	Design of potential reverse transcriptase inhibitor containing Isatin nucleus using molecular modeling studies. Bioorganic and Medicinal Chemistry, 2010, 18, 3198-3211.	3.0	33
7	Design, synthesis and pharmacological screening of novel nitric oxide donors containing 1,5-diarylpyrazolin-3-one as nontoxic NSAIDs. European Journal of Medicinal Chemistry, 2009, 44, 4622-4636.	5.5	32
8	Synthesis, antimicrobial evaluation, and molecular docking studies of novel chromone based 1,2,3-triazoles. Research on Chemical Intermediates, 2017, 43, 15-28.	2.7	32
9	Design, docking study and ADME prediction of Isatin derivatives as anti-HIV agents. Medicinal Chemistry Research, 2011, 20, 370-380.	2.4	27
10	Design, synthesis, and evaluation of anti-inflammatory, analgesic, ulcerogenicity, and nitric oxide releasing studies of novel indomethacin analogs as non-ulcerogenic derivatives. Journal of Enzyme Inhibition and Medicinal Chemistry, 2010, 25, 520-530.	5.2	26
11	Microwave-Assisted Facile Synthesis, Anticancer Evaluation and Docking Study of N-((5-(Substituted) Tj ETQq1 1 0.784314 rgBT /Ove	3.8	25
12	Investigating the Impact of Different Acrylamide (Electrophilic Warhead) on Osimertinibâ€™s Pharmacological Spectrum by Molecular Mechanic and Quantum Mechanic Approach. Combinatorial Chemistry and High Throughput Screening, 2021, 25, 149-166.	1.1	25
13	BREED based de novo hybridization approach: generating novel T790M/C797S-EGFR tyrosine kinase inhibitors to overcome the problem of mutation and resistance in non small cell lung cancer (NSCLC). Journal of Biomolecular Structure and Dynamics, 2021, 39, 2838-2856.	3.5	24
14	New amide linked dimeric 1,2,3-triazoles bearing aryloxy scaffolds as a potent antiproliferative agents and EGFR tyrosine kinase phosphorylation inhibitors. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 126618.	2.2	23
15	Synthesis, Antifungal Activity, and Docking Study of Some New 1,2,4â€triazole Analogs. Chemical Biology and Drug Design, 2011, 78, 800-809.	3.2	21
16	Synthesis, biological activity and docking study of imidazol-5-one as novel non-nucleoside HIV-1 reverse transcriptase inhibitors. Bioorganic and Medicinal Chemistry, 2012, 20, 3119-3127.	3.0	20
17	Design of selective TACE inhibitors using molecular docking studies: Synthesis and preliminary evaluation of anti-inflammatory and TACE inhibitory activity. SAR and QSAR in Environmental Research, 2015, 26, 905-923.	2.2	19
18	Synthesis and Evaluation of 1,2,3â€Triazoleâ€Containing Vinyl and Allyl Sulfones as Antiâ€Trypanosomal Agents. European Journal of Organic Chemistry, 2017, 2017, 175-185.	2.4	19

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19	Novel Oâ€Alkylated Chromones as Antimicrobial Agents: Ultrasound Mediated Synthesis, Molecular Docking and ADME Prediction. Journal of Heterocyclic Chemistry, 2017, 54, 2678-2685.	2.6	18
20	Design and synthesis of novel conformationally constrained 7,12-dihydrodibenzo[b,h][1,6] naphthyridine and 7H-Chromeno[3,2-c] quinoline derivatives as topoisomerase I inhibitors: In vitro screening, molecular docking and ADME predictions. Bioorganic Chemistry, 2021, 115, 105174.	4.1	18
21	Development of energetic pharmacophore for the designing of 1,2,3,4-tetrahydropyrimidine derivatives as selective cyclooxygenase-2 inhibitors. Journal of Computer-Aided Molecular Design, 2012, 26, 267-277.	2.9	16
22	3D QSAR studies based in silico screening of 4,5,6-triphenyl-1,2,3,4-tetrahydropyrimidine analogs for anti-inflammatory activity. European Journal of Medicinal Chemistry, 2014, 73, 233-242.	5.5	14
23	Ultrasound assisted synthesis of tetrazole based pyrazolines and isoxazolines as potent anticancer agents via inhibition of tubulin polymerization. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127592.	2.2	14
24	Structure-Based Site of Metabolism (SOM) Prediction of Ligand for CYP3A4 Enzyme: Comparison of Glide XP and Induced Fit Docking (IFD). Molecules, 2020, 25, 1622.	3.8	13
25	Synthesis and evaluation of anti-inflammatory, analgesic, ulcerogenicity and nitric oxide-releasing studies of novel ibuprofen analogs as nonulcerogenic derivatives. Medicinal Chemistry Research, 2011, 20, 795-808.	2.4	12
26	Green synthesis and biological evaluation of some new benzothiazolo [2,3-b] quinazolin-1-ones as anticancer agents. Medicinal Chemistry Research, 2014, 23, 4893-4900.	2.4	12
27	Hetero-substituted sulfonamido-benzamide hybrids as glucokinase activators: Design, synthesis, molecular docking and in-silico ADME evaluation. Journal of Molecular Structure, 2020, 1222, 128916.	3.6	12
28	Pharmaceutical analysis combined with in-silico therapeutic and toxicological profiling on zileuton and its impurities to assist in modern drug discovery. Journal of Pharmaceutical and Biomedical Analysis, 2020, 179, 112982.	2.8	11
29	3D-QSAR and docking studies of benzoyl urea derivatives as tubulin-binding agents for antiproliferative activity. Medicinal Chemistry Research, 2013, 22, 1415-1425.	2.4	10
30	DEVELOPMENT OF NEW PYRAZOLE HYBRIDS AS ANTITUBERCULAR AGENTS: SYNTHESIS, BIOLOGICAL EVALUATION AND MOLECULAR DOCKING STUDY. International Journal of Pharmacy and Pharmaceutical Sciences, 2017, 9, 50.	0.3	10
31	Use of Quantitative Structureâ€“Activity Relationship (QSAR) and ADMET prediction studies as screening methods for design of benzyl urea derivatives for anti-cancer activity. Journal of Enzyme Inhibition and Medicinal Chemistry, 2011, 26, 319-331.	5.2	9
32	Development of triple mutant T790M/C797S allosteric EGFR inhibitors: a computational approach. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5376-5398.	3.5	9
33	Synthesis, in-vitro reverse transcriptase inhibitory activity and docking study of some new imidazol-5-one analogs. Medicinal Chemistry Research, 2014, 23, 3752-3764.	2.4	7
34	Quinazolin-4-one derivatives lacking toxicity-producing attributes as glucokinase activators: design, synthesis, molecular docking, and in-silico ADMET prediction. Future Journal of Pharmaceutical Sciences, 2019, 5, .	2.8	7
35	N-Benzylation of 6-aminoflavone by reductive amination and efficient access to some novel anticancer agents via topoisomerase II inhibition. Molecular Diversity, 2021, 25, 937-948.	3.9	7
36	Strategic analyses to identify key structural features of antiviral/antimalarial compounds for their binding interactions with 3CLpro, PLpro and RdRp of SARS-CoV-2: in silico molecular docking and dynamic simulation studies. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11914-11931.	3.5	7

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37	Synthesis, Biological Evaluation, Molecular Docking Study and Acute Oral Toxicity Study of Coupled Imidazole-Pyrimidine Derivatives. Letters in Drug Design and Discovery, 2018, 15, 475-487.	0.7	7
38	One pot synthesis, in silico study and evaluation of some novel flavonoids as potent topoisomerase II inhibitors. Bioorganic and Medicinal Chemistry Letters, 2021, 40, 127916.	2.2	6
39	Synthesis and evaluation of novel sulfonamide analogues of 6/7-aminoflavones as anticancer agents via topoisomerase II inhibition. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127246.	2.2	6
40	Explorations of novel pyridine-pyrimidine hybrid phosphonate derivatives as aurora kinase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2022, 67, 128747.	2.2	6
41	Novel 2-(nitrooxy)ethyl 2-(4-(substituted phenyl)-2-((substituted phenyl)amino)thiazol-5-yl)acetate as Anti-inflammatory, Analgesic and Nitric Oxide Releasing Agents: Synthesis and Molecular Docking Studies. Anti-Inflammatory and Anti-Allergy Agents in Medicinal Chemistry, 2018, 16, 153-167.	1.1	4
42	Synthesis, Biological Evaluation and Computational Study of New Quinoline Hybrids as Antitubercular Agent. Letters in Drug Design and Discovery, 2018, 15, 914-922.	0.7	3
43	Molecular dynamic simulations based discovery and development of thiazolidin-4-one derivatives as EGFR inhibitors targeting resistance in non-small cell lung cancer (NSCLC). Journal of Biomolecular Structure and Dynamics, 2023, 41, 4696-4710.	3.5	2
44	Caesalpinia pulcherrima sarrests cell cycle and triggers reactive oxygen species-induced mitochondrial-mediated apoptosis and necroptosis via modulating estrogen and estrogen receptors. Pharmacognosy Magazine, 2019, 15, 288.	0.6	1
45	Pyridine/pyrimidine Substituted Imidazol-5-one Analogs as HIV-1 RT Inhibitors: Design, Synthesis, Docking and Molecular Dynamic Simulation Studies. Current HIV Research, 2021, 19, .	0.5	0
46	Design, Synthesis and Anti-breast Cancer Activity of Some Novel Substituted Isoxazoles as Anti-breast Cancer Agent. Anti-Cancer Agents in Medicinal Chemistry, 2018, 18, 1009-1015.	1.7	0