Umesh Yadava

List of Publications by Year
in descending order

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56	986	471509	477307
papers	citations	17	29
		h-index	g-index

57	57	57	1245
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	DFT calculations on molecular structure, MEP and HOMO-LUMO study of 3-phenyl-1-(methyl-sulfonyl)-1H-pyrazolo[3,4-d]pyrimidine-4-amine. Materials Today: Proceedings, 2022, 49, 3056-3060.	1.8	9
2	SARS-CoV-2 M^{pro}inhibitors: identification of anti-SARS-CoV-2 M^{pro}compounds from FDA approved drugs. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2769-2784.	3.5	41
3	Structure-based screening and validation of bioactive compounds as Zika virus methyltransferase (MTase) inhibitors through first-principle density functional theory, classical molecular simulation and QM/MM affinity estimation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2338-2351.	3.5	30
4	Anti-dengue infectivity evaluation of bioflavonoid from Azadirachta indica by dengue virus serine protease inhibition. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1417-1430.	3.5	38
5	Exploration of natural compounds with anti-SARS-CoV-2 activityviainhibition of SARS-CoV-2 Mpro. Briefings in Bioinformatics, 2021, 22, 1361-1377.	6.5	108
6	Explorations on the electronic structure and spectroscopic IR assignments of 5-methyl-2-(2-oxopropyl)-pyrazolo[5,1-b]quinazolin-9(3H)-one molecule. IOP SciNotes, 2021, 2, 014004.	0.8	0
7	Structure-Based Identification of Natural Products as SARS-CoV-2 Mpro Antagonist from Echinacea angustifolia Using Computational Approaches. Viruses, 2021, 13, 305.	3.3	25
8	Synthesis, biological evaluation and molecular docking studies of novel quinazolinones as antitubercular and antimicrobial agents. Bioorganic Chemistry, 2021, 108, 104611.	4.1	8
9	Drug repurposing for ligand-induced rearrangement of Sirt2 active site-based inhibitors via molecular modeling and quantum mechanics calculations. Scientific Reports, 2021, 11, 10169.	3.3	42
10	Determination of tyrosinase-cyanidin-3-O-glucoside and (â˜'/+)-catechin binding modes reveal mechanistic differences in tyrosinase inhibition. Scientific Reports, 2021, 11, 24494.	3.3	10
11	Computational investigations and molecular dynamics simulations envisioned for potent antioxidant and anticancer drugs using indole-chalcone-triazole hybrids. DNA Repair, 2020, 86, 102765.	2.8	7
12	Computational and In Vitro Investigation of (-)-Epicatechin and Proanthocyanidin B2 as Inhibitors of Human Matrix Metalloproteinase 1. Biomolecules, 2020, 10, 1379.	4.0	13
13	Speculative analysis on the electronic structure, IR assignments and molecular docking of N-{4-[(4-amino-3-phenyl-1H-pyrazolo[3,4-d]pyrimidin-1-yl)sulfonyl]phenyl}acetamide, an anti-amoebic agent. Heliyon, 2020, 6, e04176.	3.2	2
14	Density functional theory and molecular dynamics simulation support Ganoderma lucidum triterpenoids as broad range antagonist of matrix metalloproteinases. Journal of Molecular Liquids, 2020, 311, 113322.	4.9	13
15	Electronic structure and vibrational assignments of 2,5-bis[4-(n-cyclobutyldiaminomethyl)phenyl]furan. IOP SciNotes, 2020, 1, 024005.	0.8	1
16	Computational aided mechanistic understanding of Camellia sinensis bioactive compounds against coâ€chaperone p23 as potential anticancer agent. Journal of Cellular Biochemistry, 2019, 120, 19064-19075.	2.6	15
17	Investigation of DNA binding and molecular docking propensity of phthalimide derivatives: in vitro antibacterial and antioxidant assay. Journal of Analytical Science and Technology, 2019, 10, .	2.1	14
18	Evaluation of caffeine as inhibitor against collagenase, elastase and tyrosinase using in silico and in vitro approach. Journal of Enzyme Inhibition and Medicinal Chemistry, 2019, 34, 927-936.	5.2	53

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19	Investigations on bisamidine derivatives as novel minor groove binders with the dodecamer 5â€²(CGCGAATTCGCG)3â€². Journal of Molecular Liquids, 2019, 280, 135-152.	4.9	8
20	Discovery of Ganoderma lucidum triterpenoids as potential inhibitors against Dengue virus NS2B-NS3 protease. Scientific Reports, 2019, 9, 19059.	3.3	75
21	Synthesis and mechanistic studies of diketo acids and their bioisosteres as potential antibacterial agents. European Journal of Medicinal Chemistry, 2019, 163, 67-82.	5.5	7
22	Ribonucleotide reductase as a drug target against drug resistance Mycobacterium leprae : A molecular docking study. Infection, Genetics and Evolution, 2018, 60, 58-65.	2.3	7
23	Co-chaperon p23 inhibitors: Identification of anticancer compounds from traditional Chinese medicine database. Gene Reports, 2018, 10, 135-140.	0.8	2
24	Natural Product-Based 1,2,3-Triazole/Sulfonate Analogues as Potential Chemotherapeutic Agents for Bacterial Infections. ACS Omega, 2018, 3, 6912-6930.	3.5	46
25	Search algorithms and scoring methods in protein-ligand docking. Endocrinology&Metabolism International Journal, 2018, 6, .	0.1	7
26	Novel anti-tubulin agents from plant and marine origins: insight from a molecular modeling and dynamics study. RSC Advances, 2017, 7, 15917-15925.	3.6	16
27	Efficient synthesis of novel N-substituted 2-carboxy-4-quinolones via lithium bis(trimethylsilyl)amide (LiHMDS)-induced in situ cyclocondensation reaction. RSC Advances, 2017, 7, 11367-11372.	3.6	10
28	Anti-leishmanial and cytotoxic activities of amino acid-triazole hybrids: Synthesis, biological evaluation, molecular docking and in silico physico-chemical properties. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 1886-1891.	2.2	19
29	Electronic structure, vibrational assignments and simulation studies with A/T rich DNA duplex of an aromatic bis-amidine derivative. DNA Repair, 2017, 60, 9-17.	2.8	13
30	Study the effect of heat processing on the vitamin C of some fruits. International Journal of Food and Allied Sciences, 2017, 3, 36.	0.4	2
31	Effect of Polarization of Ligand Charges and Estimation of MM/GBSA Binding Free Energies of Some Pyrazolo[3,4-d]pyrimidine Inhibitors of Mycobacterium Tuberculosis in View of Experimental Results. Current Enzyme Inhibition, 2017, 13, .	0.4	1
32	Characterizations of solute-binding proteins by DSF scanning and crystallography. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C156-C156.	0.1	0
33	Structure of an ABC transporter solute-binding protein specific for the amino sugars glucosamine and galactosamine. Acta Crystallographica Section F, Structural Biology Communications, 2016, 72, 467-472.	0.8	5
34	QSAR study of some pyrazolo[3,4-d]pyrimidine derivatives as the c-Src inhibitors. AIP Conference Proceedings, 2016, , .	0.4	0
35	Molecular dynamics simulation of hydrated d(CGGGTACCCG)4as a four-way DNA Holliday junction and comparison with the crystallographic structure. Molecular Simulation, 2016, 42, 25-30.	2.0	8
36	Monocyclic Î²-lactam and unexpected oxazinone formation: synthesis, crystal structure, docking studies and antibacterial evaluation. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 834-852.	5.2	15

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37	An unusual conformational change in the folded trimethylene/leonard linker pyrazolo[3,4-d]pyrimidine analogue of the theophylline compound due to structural changes. Journal of Structural Chemistry, 2015, 56, 1437-1440.	1.0	0
38	Synthesis, QSAR and anticandidal evaluation of 1,2,3-triazoles derived from naturally bioactive scaffolds. European Journal of Medicinal Chemistry, 2015, 93, 246-254.	5.5	63
39	Stabilization of Microtubules by Taxane Diterpenoids: Insight from Docking and MD simulations. Journal of Biological Physics, 2015, 41, 117-133.	1.5	40
40	Pyrazolo[3,4-d]pyrimidines as novel inhibitors of O-acetyl-l-serine sulfhydrylase of Entamoeba histolytica: an in silico study. Journal of Molecular Modeling, 2015, 21, 96.	1.8	28
41	Diketo acids and their amino acid/dipeptidic analogues as promising scaffolds for the development of bacterial methionine aminopeptidase inhibitors. RSC Advances, 2015, 5, 34173-34183.	3.6	20
42	Theoretical explorations on the molecular structure and IR frequencies of 3-phenyl-1-tosyl-1H-pyrazolo[3,4-d]pyrimidin-4-amine in view of experimental results. Journal of Molecular Liquids, 2015, 212, 325-330.	4.9	14
43	Pyrazolo[3,4-d]pyrimidines as the inhibitors of mycobacterial Î²-oxidation trifunctional enzyme. Medicinal Chemistry Research, 2015, 24, 4002-4015.	2.4	5
44	Synthesis, spectral characterization and antimicrobial studies of nano-sized oxovanadium(IV) complexes with Schiff bases derived from 5-(phenyl/substituted phenyl)-2-hydrazino-1,3,4-thiadiazole and indoline-2,3-dione. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 125, 189-194.	3.9	18
45	Molecular dynamics simulation of DNA duplex, analog of PPT (polypurine tract), its conformation and hydration: a theoretical study. Medicinal Chemistry Research, 2014, 23, 280-286.	2.4	9
46	Determination of distances and sizes of visible objects using a plane transparent glass plate. Results in Physics, 2014, 4, 83-87.	4.1	1
47	Docking and Molecular Dynamics Simulations of Pyrazolo[3,4-d]Pyrimidine-DNA Complexes. Advanced Science Letters, 2014, 20, 1637-1643.	0.2	2
48	Molecular modeling and structural studies of 12-mer immobile four-way DNA junction in solution. Bioinformation, 2014, 10, 394-400.	0.5	2
49	Pyrazolo[3,4-d]pyrimidines as inhibitor of anti-coagulation and inflammation activities of phospholipase A 2 : insight from molecular docking studies. Journal of Biological Physics, 2013, 39, 419-438.	1.5	33
50	2,2â€²-Bipyridyl-acetylphenolato mixed ligand copper(II) complexes: syntheses, characterizations and catalytic activity in styrene epoxidation. Journal of Coordination Chemistry, 2013, 66, 66-76.	2.2	7
51	A comparison of crystallographic and DFT optimized geometries on two taxane diterpenoids and docking studies with phospholipase A2. Medicinal Chemistry Research, 2012, 21, 2162-2168.	2.4	19
52	Gas-phase conformational and intramolecular Ï€â€“Ï€ interaction studies on some pyrazolo[3,4-d]pyrimidine derivatives. Computational and Theoretical Chemistry, 2011, 977, 134-139.	2.5	27
53	Theoretical investigations on molecular structure and IR frequencies of 4-n-nonyl-4â€²-cyanobiphenyl in light of experimental results. Journal of Molecular Liquids, 2010, 156, 187-190.	4.9	9
54	5,8-Diethyl-6,9-dithioxo-2,3,5,6,8,9-hexahydro-1H-3a,5,8,9a-tetraazaphenalene-4,7-dione. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, o4991-o4993.	0.2	0

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55	Fine tuning of folded conformation by change of substituents: 1H NMR and crystallographic evidence for folded conformation due to arene interactions in pyrazolo[3,4-d]pyrimidine core based â€˜propylene linkerâ€™ compounds. Journal of Molecular Structure, 2005, 750, 179-185.	3.6	15
56	Guggulsterone E, a lipid-lowering agent fromCommiphora mukul. Acta Crystallographica Section E: Structure Reports Online, 2001, 57, o285-o286.	0.2	4