Samir Chtita

List of Publications by Year
in descending order

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68	1,101	361045	500791
papers	citations	20	28
		h-index	g-index

68	68	68	553
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	QSAR, molecular docking and ADMET properties in silico studies of novel 4,5,6,7-tetrahydrobenzo[D]-thiazol-2-Yl derivatives derived from dimedone as potent anti-tumor agents through inhibition of C-Met receptor tyrosine kinase. Heliyon, 2021, 7, e07463.	1.4	53
2	Identification of a novel dual-target scaffold for 3CLpro and RdRp proteins of SARS-CoV-2 using 3D-similarity search, molecular docking, molecular dynamics and ADMET evaluation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4522-4535.	2.0	49
3	Identification of potent inhibitors of NEK7 protein using a comprehensive computational approach. Scientific Reports, 2022, 12, 6404.	1.6	48
4	Virtual screening in drug-likeness and structure/activity relationship of pyridazine derivatives as Anti-Alzheimer drugs. Journal of King Saud University - Science, 2019, 31, 595-601.	1.6	41
5	Design of novel benzimidazole derivatives as potential Î±-amylase inhibitors using QSAR, pharmacokinetics, molecular docking, and molecular dynamics simulation studies. Journal of Molecular Modeling, 2022, 28, 106.	0.8	41
6	QSAR study of unsymmetrical aromatic disulfides as potent avian SARS-CoV main protease inhibitors using quantum chemical descriptors and statistical methods. Chemometrics and Intelligent Laboratory Systems, 2021, 210, 104266.	1.8	40
7	Discovery of Potent SARS-CoV-2 Inhibitors from Approved Antiviral Drugs via Docking and Virtual Screening. Combinatorial Chemistry and High Throughput Screening, 2021, 24, 441-454.	0.6	39
8	Combined molecular docking and dynamics simulations studies of natural compounds as potent inhibitors against SARS-CoV-2 main protease. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11264-11273.	2.0	37
9	Cameroonian medicinal plants as potential candidates of SARS-CoV-2 inhibitors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 8615-8629.	2.0	36
10	In silico detection of potential inhibitors from vitamins and their derivatives compounds against SARS-CoV-2 main protease by using molecular docking, molecular dynamic simulation and ADMET profiling. Journal of Molecular Structure, 2022, 1258, 132652.	1.8	36
11	Camphor, Artemisinin and Sumac Phytochemicals as inhibitors against COVID-19: Computational approach. Computers in Biology and Medicine, 2021, 136, 104758.	3.9	33
12	Quantitative structureâ€“activity relationship studies of dibenzo[a,d]cycloalkenimine derivatives for non-competitive antagonists ofN-methyl-<scp>d</scp>-aspartate based on density functional theory with electronic and topological descriptors. Journal of Taibah University for Science, 2015, 9, 143-154.	1.1	31
13	Combined docking methods and molecular dynamics to identify effective antiviral 2, 5-diaminobenzophenonederivatives against SARS-CoV-2. Journal of King Saud University - Science, 2021, 33, 101352.	1.6	30
14	Design, synthesis, characterization,in vitroscreening, molecular docking, 3D-QSAR, and ADME-Tox investigations of novel pyrazole derivatives as antimicrobial agents. New Journal of Chemistry, 2022, 46, 2747-2760.	1.4	30
15	QSAR study of anti-Human African Trypanosomiasis activity for 2-phenylimidazopyridines derivatives using DFT and Lipinski's descriptors. Heliyon, 2019, 5, e01304.	1.4	29
16	QSAR study of N-substituted oseltamivir derivatives as potent avian influenza virus H5N1 inhibitors using quantum chemical descriptors and statistical methods. New Journal of Chemistry, 2020, 44, 1747-1760.	1.4	26
17	The inhibitory activity of aldose reductase of flavonoid compounds: Combining DFT and QSAR calculations. Journal of Taibah University for Science, 2016, 10, 534-542.	1.1	24
18	Combined 3D-QSAR and molecular docking study on 7,8-dialkyl-1,3-diaminopyrrolo-[3,2-f] Quinazoline series compounds to understand the binding mechanism of DHFR inhibitors. Journal of Molecular Structure, 2017, 1139, 319-327.	1.8	24

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19	Furanone derivatives as new inhibitors of CDC7 kinase: development of structure activity relationship model using 3D QSAR, molecular docking, and in silico ADMET. Structural Chemistry, 2018, 29, 1031-1043.	1.0	23
20	3D-QSAR, ADME-Tox, and molecular docking of semisynthetic triterpene derivatives as antibacterial and insecticide agents. Structural Chemistry, 2022, 33, 1063-1084.	1.0	23
21	Investigation of Antileishmanial Activities of Acridines Derivatives against Promastigotes and Amastigotes Form of Parasites Using Quantitative Structure Activity Relationship Analysis. Advances in Physical Chemistry, 2016, 2016, 1-16.	2.0	22
22	QSAR analysis of the toxicity of phenols and thiophenols using MLR and ANN. Journal of Taibah University for Science, 2017, 11, 1-10.	1.1	22
23	2Dâ€QSAR and molecular docking studies of carbamate derivatives to discover novel potent antiâ€butyrylcholinesterase agents for Alzheimer's disease treatment. Bulletin of the Korean Chemical Society, 2022, 43, 277-292.	1.0	22
24	QSPR studies of 9-aniliioacridine derivatives for their DNA drug binding properties based on density functional theory using statistical methods: Model, validation and influencing factors. Journal of Taibah University for Science, 2016, 10, 868-876.	1.1	21
25	Rational identification of small molecules derived from 9,10-dihydrophenanthrene as potential inhibitors of 3CLpro enzyme for COVID-19 therapy: a computer-aided drug design approach. Structural Chemistry, 2022, 33, 1667-1690.	1.0	21
26	Combined 3D-QSAR and Molecular Docking Analysis of Thienopyrimidine Derivatives as Staphylococcus aureus Inhibitors. Acta Chimica Slovenica, 2021, 68, 289-303.	0.2	18
27	Molecular docking analysis of N-substituted oseltamivir derivatives with the SARS-Cov-2 main protease. Bioinformation, 2020, 16, 404-410.	0.2	17
28	Theoretical study of photovoltaic performances of Ru, Rh and Ir half sandwich complexes containing N,N chelating ligands in Dye-Sensitized Solar Cells (DSSCs). DFT and TD-DFT investigation. Computational and Theoretical Chemistry, 2022, 1209, 113630.	1.1	16
29	In silico investigation of phytoconstituents from Cameroonian medicinal plants towards COVID-19 treatment. Structural Chemistry, 2022, 33, 1799-1813.	1.0	15
30	Research of new acetylcholinesterase inhibitors based on QSAR and molecular docking studies of benzene-based carbamate derivatives. Structural Chemistry, 2022, 33, 1935-1946.	1.0	15
31	Investigation of indirubin derivatives: a combination of 3D-QSAR, molecular docking, and ADMET towards the design of new DRAK2 inhibitors. Structural Chemistry, 2018, 29, 1609-1622.	1.0	14
32	QSAR modeling, molecular docking, ADMET prediction and molecular dynamics simulations of some 6-arylquinazolin-4-amine derivatives as DYRK1A inhibitors. Journal of Molecular Structure, 2022, 1258, 132659.	1.8	14
33	Multi-combined 3D-QSAR, docking molecular and ADMET prediction of 5-azaindazole derivatives as LRRK2 tyrosine kinase inhibitors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1285-1298.	2.0	13
34	Synthesis, crystal structure, IR, Raman-spectroscopy and DFT computation of monostrontium phosphate monohydrate, Sr(H₂PO₄)₂Â·H₂O. Journal of Coordination Chemistry, 2020, 73, 2328-2346.	0.8	13
35	Analysis and prediction pathways of natural products and their cytotoxicity against HeLa cell line protein using docking, molecular dynamics and ADMET. Journal of Biomolecular Structure and Dynamics, 2023, 41, 765-777.	2.0	13
36	Computer aided drug design based on 3D-QSAR and molecular docking studies of 5-(1H-indol-5-yl)-1,3,4-thiadiazol-2-amine derivatives as PIM2 inhibitors: a proposal to chemists. In Silico Pharmacology, 2018, 6, 5.	1.8	12

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37	Design and Prediction of ADME/Tox Properties of Novel Magnolol Derivatives as Anticancer Agents for NSCLC Using 3D-QSAR, Molecular Docking, MOLCAD and MM-GBSA Studies. Letters in Drug Design and Discovery, 2023, 20, 545-569.	0.4	12
38	QTAIM and IRC studies for the evaluation of activation energy on the C=P, C=N and C=O Diels-Alder reaction. Heliyon, 2020, 6, e04655.	1.4	10
39	Structural characterization and QSAR modeling of 1,2,4-triazole derivatives as Î±-glucosidase inhibitors. New Journal of Chemistry, 2021, 45, 1253-1261.	1.4	10
40	QSAR study and rustic ligand-based virtual screening in a search for aminooxadiazole derivatives as PIM1 inhibitors. Chemistry Central Journal, 2018, 12, 32.	2.6	9
41	Predictive modelling of the LD50 activities of coumarin derivatives using neural statistical approaches: Electronic descriptor-based DFT. Journal of Taibah University for Science, 2016, 10, 451-461.	1.1	8
42	QSPR study of the retention/release property of odorant molecules in pectin gels using statistical methods. Journal of Taibah University for Science, 2017, 11, 1030-1046.	1.1	8
43	Artificial neural <scp>networkâ€based</scp> quantitative structureâ€“activity relationships model and molecular docking for virtual screening of novel potent acetylcholinesterase inhibitors. Journal of the Chinese Chemical Society, 2021, 68, 1379-1399.	0.8	8
44	Combining DFT and QSAR studies for predicting psychotomimetic activity of substituted phenethylamines using statistical methods. Journal of Taibah University for Science, 2016, 10, 787-796.	1.1	7
45	Discovery of Phenylcarbamoylazinane-1,2,4-Triazole Amides Derivatives as the Potential Inhibitors of Aldo-Keto Reductases (AKR1B1 & AKRB10): Potential Lead Molecules for Treatment of Colon Cancer. Molecules, 2022, 27, 3981.	1.7	7
46	Molecular Docking and 3D-QSAR Studies on 7-azaindole Derivatives as Inhibitors of Trk A: A Strategic Design in Novel Anticancer Agents. Letters in Drug Design and Discovery, 2018, 15, 1211-1223.	0.4	6
47	Design of hydroxyl- and thioether-functionalized iron-platinum dimetallacyclopentenone complexes. Crystal and electronic structures, Hirshfeld and docking analyses and anticancer activity evaluated by inÂsilico simulation. Journal of Molecular Structure, 2022, 1251, 131979.	1.8	6
48	QSAR Modelling of Peptidomimetic Derivatives towards HKU4-CoV 3CLpro Inhibitors against MERS-CoV. Chemistry, 2021, 3, 391-401.	0.9	5
49	Combining DFT and QSAR computation to predict the interaction of flavonoids with the GABA (A) receptor using electronic and topological descriptors. Journal of Taibah University for Science, 2017, 11, 422-433.	1.1	4
50	Study of interactions between odorant molecules and the hOR1G1 olfactory receptor by molecular modeling. Egyptian Journal of Ear, Nose, Throat and Allied Sciences, 2017, 18, 257-265.	0.0	4
51	Structural basis of pyrazolopyrimidine derivatives as CAMKIIÎ´ kinase inhibitors: insights from 3D QSAR, docking studies and in silico ADMET evaluation. Chemical Papers, 2018, 72, 2833-2847.	1.0	4
52	QSPR Study of the Retention/release Property of Odorant Molecules in Water Using Statistical Methods. Orbital, 2017, 9, .	0.1	4
53	Quantitative Structureâ€“Activity Relationship Studies of Anticancer Activity for Isatin (1H-indole-2,3-dione) Derivatives Based on Density Functional Theory. International Journal of Quantitative Structure-Property Relationships, 2017, 2, 90-115.	1.1	3
54	QSAR Study of (5-Nitroheteroaryl-1,3,4-Thiadiazole-2-yl) Piperazinyl Derivatives to Predict New Similar Compounds as Antileishmanial Agents. Advances in Physical Chemistry, 2018, 2018, 1-10.	2.0	3

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55	QSPR Study of the Retention/Release Property of Odorant Molecules in Water, Dairy and Pectin gels. Materials Today: Proceedings, 2019, 13, 621-629.	0.9	3
56	QSAR and DFT studies of some Tacrine-hydroxamate derivatives as inhibitors of Cholinesterase (AChEs) in the treatment of Alzheimer's disease. Letters in Drug Design and Discovery, 2022, 19, .	0.4	3
57	QSAR studies on PIM1 and PIM2 inhibitors using statistical methods: a rustic strategy to screen for 5-(1H-indol-5-yl)-1,3,4-thiadiazol analogues and predict their PIM inhibitory activity. Chemistry Central Journal, 2017, 11, 41.	2.6	2
58	QSPR and DFT Studies on the Melting Point of Carbocyclic Nitroaromatic Compounds. , 2017, 07, .		2
59	2D-QSPR Study of Olfactive Thresholds for Pyrazine Derivatives Using DFT and Statistical Methods. Emerging Science Journal, 2019, 3, 179-186.	1.4	2
60	Quantitative Structure-Activity Relationships of 1.2.3 Triazole Derivatives as Aromatase Inhibition Activity. Turkish Computational and Theoretical Chemistry, 2020, 4, 1-11.	0.5	2
61	Combined 3D-{QSAR} and Molecular Docking Analysis of Thienopyrimidine Derivatives as Staphylococcus aureus Inhibitors. Acta Chimica Slovenica, 2021, 68, 289-303.	0.2	2
62	QSAR Modeling of Styrylquinoline Derivatives as HIV-1 Integrase Inhibitors. Current Chemical Biology, 2022, 16, 123-129.	0.2	2
63	Synthesis, crystal structure, IR spectroscopy, and DFT computation of the new variety of 2-carboxyanilinium dihydrogen phosphate (C7H8NO2+. H2PO4â^'). Journal of Molecular Structure, 2021, 1242, 130707.	1.8	1
64	QSAR Studies of Toxicity Towards Monocytes with (1,3-benzothiazol-2-yl) amino-9-(10H)-acridinone Derivatives Using Electronic Descriptors. Orbital, 2015, 7, .	0.1	1
65	Quantitative structure - toxicity relationship studies of aromatic aldehydes to Tetrahymena pyriformis base d on electronic and topological descriptors. Journal of Materials and Environmental Science, 2018, 9, 256-265.	0.5	1
66	Neuropharmacological investigation, ultra-high performance liquid chromatography analysis, and in silico studies of Phyla nodiflora.. Journal of Physiology and Pharmacology, 2021, 72, .	1.1	1
67	Synthesis, crystal structure, vibrational study and DFT computation of barium dihydrogenomonophosphate Ba(H₂PO₄)₂. Acta Crystallographica Section A: Foundations and Advances, 2021, 77, C804-C804.	0.0	0
68	QSAR, molecular docking and ADMET studies of quinoline, isoquinoline and quinazoline derivatives against Plasmodium falciparum malaria. Structural Chemistry, 2023, 34, 585-603.	1.0	0