

Samir Chtita

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/8303481/publications.pdf>

Version: 2024-02-01

68
papers

1,101
citations

361045

20
h-index

500791

28
g-index

68
all docs

68
docs citations

68
times ranked

553
citing authors

#	ARTICLE	IF	CITATIONS
1	Analysis and prediction pathways of natural products and their cytotoxicity against HeLa cell line protein using docking, molecular dynamics and ADMET. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 765-777.	2.0	13
2	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. <i>Letters in Drug Design and Discovery</i> , 2023, 20, 545-569.	0.4	12
3	QSAR, molecular docking and ADMET studies of quinoline, isoquinoline and quinazoline derivatives against <i>Plasmodium falciparum</i> malaria. <i>Structural Chemistry</i> , 2023, 34, 585-603.	1.0	0
4	Multi-combined 3D-QSAR, docking molecular and ADMET prediction of 5-azaindazole derivatives as LRRK2 tyrosine kinase inhibitors. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 1285-1298.	2.0	13
5	Cameroonian medicinal plants as potential candidates of SARS-CoV-2 inhibitors. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 8615-8629.	2.0	36
6	Combined molecular docking and dynamics simulations studies of natural compounds as potent inhibitors against SARS-CoV-2 main protease. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 11264-11273.	2.0	37
7	Design of hydroxyl- and thioether-functionalized iron-platinum dimetallacyclopentenone complexes. Crystal and electronic structures, Hirshfeld and docking analyses and anticancer activity evaluated by <i>in silico</i> simulation. <i>Journal of Molecular Structure</i> , 2022, 1251, 131979.	1.8	6
8	Design, synthesis, characterization, <i>in vitro</i> screening, molecular docking, 3D-QSAR, and ADME-Tox investigations of novel pyrazole derivatives as antimicrobial agents. <i>New Journal of Chemistry</i> , 2022, 46, 2747-2760.	1.4	30
9	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. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113630.	1.1	16
10	3D-QSAR, ADME-Tox, and molecular docking of semisynthetic triterpene derivatives as antibacterial and insecticide agents. <i>Structural Chemistry</i> , 2022, 33, 1063-1084.	1.0	23
11	Design of novel benzimidazole derivatives as potential α -amylase inhibitors using QSAR, pharmacokinetics, molecular docking, and molecular dynamics simulation studies. <i>Journal of Molecular Modeling</i> , 2022, 28, 106.	0.8	41
12	QSAR Modeling of Styrylquinoline Derivatives as HIV-1 Integrase Inhibitors. <i>Current Chemical Biology</i> , 2022, 16, 123-129.	0.2	2
13	QSAR modeling, molecular docking, ADMET prediction and molecular dynamics simulations of some 6-arylquinazolin-4-amine derivatives as DYRK1A inhibitors. <i>Journal of Molecular Structure</i> , 2022, 1258, 132659.	1.8	14
14	<i>In silico</i> 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. <i>Journal of Molecular Structure</i> , 2022, 1258, 132652.	1.8	36
15	2D-QSAR and molecular docking studies of carbamate derivatives to discover novel potent anti-acetylcholinesterase agents for Alzheimer's disease treatment. <i>Bulletin of the Korean Chemical Society</i> , 2022, 43, 277-292.	1.0	22
16	Identification of potent inhibitors of NEK7 protein using a comprehensive computational approach. <i>Scientific Reports</i> , 2022, 12, 6404.	1.6	48
17	<i>In silico</i> investigation of phytoconstituents from Cameroonian medicinal plants towards COVID-19 treatment. <i>Structural Chemistry</i> , 2022, 33, 1799-1813.	1.0	15
18	QSAR and DFT studies of some Tacrine-hydroxamate derivatives as inhibitors of Cholinesterase (AChEs) in the treatment of Alzheimer's disease. <i>Letters in Drug Design and Discovery</i> , 2022, 19, .	0.4	3

#	ARTICLE	IF	CITATIONS
19	Research of new acetylcholinesterase inhibitors based on QSAR and molecular docking studies of benzene-based carbamate derivatives. <i>Structural Chemistry</i> , 2022, 33, 1935-1946.	1.0	15
20	Discovery of Phenylcarbamoylazinane-1,2,4-Triazole Amides Derivatives as the Potential Inhibitors of Aldo-Keto Reductases (AKR1B1 & AKB10): Potential Lead Molecules for Treatment of Colon Cancer. <i>Molecules</i> , 2022, 27, 3981.	1.7	7
21	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. <i>Structural Chemistry</i> , 2022, 33, 1667-1690.	1.0	21
22	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. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 4522-4535.	2.0	49
23	Structural characterization and QSAR modeling of 1,2,4-triazole derivatives as α -glucosidase inhibitors. <i>New Journal of Chemistry</i> , 2021, 45, 1253-1261.	1.4	10
24	Discovery of Potent SARS-CoV-2 Inhibitors from Approved Antiviral Drugs via Docking and Virtual Screening. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2021, 24, 441-454.	0.6	39
25	QSAR study of unsymmetrical aromatic disulfides as potent avian SARS-CoV main protease inhibitors using quantum chemical descriptors and statistical methods. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2021, 210, 104266.	1.8	40
26	QSAR Modelling of Peptidomimetic Derivatives towards HKU4-CoV 3CLpro Inhibitors against MERS-CoV. <i>Chemistry</i> , 2021, 3, 391-401.	0.9	5
27	Combined docking methods and molecular dynamics to identify effective antiviral 2,5-diaminobenzophenone derivatives against SARS-CoV-2. <i>Journal of King Saud University - Science</i> , 2021, 33, 101352.	1.6	30
28	Artificial neural network-based quantitative structure-activity relationships model and molecular docking for virtual screening of novel potent acetylcholinesterase inhibitors. <i>Journal of the Chinese Chemical Society</i> , 2021, 68, 1379-1399.	0.8	8
29	Combined 3D-QSAR and Molecular Docking Analysis of Thienopyrimidine Derivatives as <i>Staphylococcus aureus</i> Inhibitors. <i>Acta Chimica Slovenica</i> , 2021, 68, 289-303.	0.2	18
30	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. <i>Heliyon</i> , 2021, 7, e07463.	1.4	53
31	Camphor, Artemisinin and Sumac Phytochemicals as inhibitors against COVID-19: Computational approach. <i>Computers in Biology and Medicine</i> , 2021, 136, 104758.	3.9	33
32	Synthesis, crystal structure, IR spectroscopy, and DFT computation of the new variety of 2-carboxyanilinium dihydrogen phosphate ($C_7H_8NO_2^+ \cdot H_2PO_4^-$). <i>Journal of Molecular Structure</i> , 2021, 1242, 130707.	1.8	1
33	Combined 3D-QSAR and Molecular Docking Analysis of Thienopyrimidine Derivatives as <i>Staphylococcus aureus</i> Inhibitors. <i>Acta Chimica Slovenica</i> , 2021, 68, 289-303.	0.2	2
34	Synthesis, crystal structure, vibrational study and DFT computation of barium dihydrogenomonophosphate $Ba(H_2PO_4)_2$. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2021, 77, C804-C804.	0.0	0
35	Neuropharmacological investigation, ultra-high performance liquid chromatography analysis, and in silico studies of <i>Phyllanthus nodiflora</i> . <i>Journal of Physiology and Pharmacology</i> , 2021, 72, .	1.1	1
36	QSAR study of <i>N</i> -substituted oseltamivir derivatives as potent avian influenza virus H5N1 inhibitors using quantum chemical descriptors and statistical methods. <i>New Journal of Chemistry</i> , 2020, 44, 1747-1760.	1.4	26

#	ARTICLE	IF	CITATIONS
37	QTAIM and IRC studies for the evaluation of activation energy on the C=P, C=N and C=O Diels-Alder reaction. <i>Heliyon</i> , 2020, 6, e04655.	1.4	10
38	Synthesis, crystal structure, IR, Raman-spectroscopy and DFT computation of monostrontium phosphate monohydrate, Sr(H ₂ PO ₄) ₂ ·H ₂ O. <i>Journal of Coordination Chemistry</i> , 2020, 73, 2328-2346.	0.8	13
39	Molecular docking analysis of N-substituted oseltamivir derivatives with the SARS-Cov-2 main protease. <i>Bioinformatics</i> , 2020, 16, 404-410.	0.2	17
40	Quantitative Structure-Activity Relationships of 1.2.3 Triazole Derivatives as Aromatase Inhibition Activity. <i>Turkish Computational and Theoretical Chemistry</i> , 2020, 4, 1-11.	0.5	2
41	QSPR Study of the Retention/Release Property of Odorant Molecules in Water, Dairy and Pectin gels. <i>Materials Today: Proceedings</i> , 2019, 13, 621-629.	0.9	3
42	QSAR study of anti-Human African Trypanosomiasis activity for 2-phenylimidazopyridines derivatives using DFT and Lipinski's descriptors. <i>Heliyon</i> , 2019, 5, e01304.	1.4	29
43	Virtual screening in drug-likeness and structure/activity relationship of pyridazine derivatives as Anti-Alzheimer drugs. <i>Journal of King Saud University - Science</i> , 2019, 31, 595-601.	1.6	41
44	2D-QSPR Study of Olfactive Thresholds for Pyrazine Derivatives Using DFT and Statistical Methods. <i>Emerging Science Journal</i> , 2019, 3, 179-186.	1.4	2
45	Furanone derivatives as new inhibitors of CDC7 kinase: development of structure activity relationship model using 3D QSAR, molecular docking, and in silico ADMET. <i>Structural Chemistry</i> , 2018, 29, 1031-1043.	1.0	23
46	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. <i>In Silico Pharmacology</i> , 2018, 6, 5.	1.8	12
47	Molecular Docking and 3D-QSAR Studies on 7-azaindole Derivatives as Inhibitors of Trk A: A Strategic Design in Novel Anticancer Agents. <i>Letters in Drug Design and Discovery</i> , 2018, 15, 1211-1223.	0.4	6
48	QSAR Study of (5-Nitroheteroaryl-1,3,4-Thiadiazole-2-yl) Piperazinyl Derivatives to Predict New Similar Compounds as Antileishmanial Agents. <i>Advances in Physical Chemistry</i> , 2018, 2018, 1-10.	2.0	3
49	Structural basis of pyrazolopyrimidine derivatives as CAMKII β kinase inhibitors: insights from 3D QSAR, docking studies and in silico ADMET evaluation. <i>Chemical Papers</i> , 2018, 72, 2833-2847.	1.0	4
50	QSAR study and rustic ligand-based virtual screening in a search for aminooxadiazole derivatives as PIM1 inhibitors. <i>Chemistry Central Journal</i> , 2018, 12, 32.	2.6	9
51	Investigation of indirubin derivatives: a combination of 3D-QSAR, molecular docking, and ADMET towards the design of new DRAX2 inhibitors. <i>Structural Chemistry</i> , 2018, 29, 1609-1622.	1.0	14
52	Quantitative structure - toxicity relationship studies of aromatic aldehydes to <i>Tetrahymena pyriformis</i> based on electronic and topological descriptors. <i>Journal of Materials and Environmental Science</i> , 2018, 9, 256-265.	0.5	1
53	QSAR analysis of the toxicity of phenols and thiophenols using MLR and ANN. <i>Journal of Taibah University for Science</i> , 2017, 11, 1-10.	1.1	22
54	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. <i>Journal of Molecular Structure</i> , 2017, 1139, 319-327.	1.8	24

#	ARTICLE	IF	CITATIONS
55	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
56	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
57	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
58	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
59	Quantitative Structure-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
60	QSPR and DFT Studies on the Melting Point of Carbocyclic Nitroaromatic Compounds. , 2017, 07, .		2
61	QSPR Study of the Retention/release Property of Odorant Molecules in Water Using Statistical Methods. Orbital, 2017, 9, .	0.1	4
62	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
63	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
64	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
65	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
66	QSPR studies of 9-anilinoacridine 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
67	Quantitative structure-activity relationship studies of dibenzo[a,d]cycloalkenimine derivatives for non-competitive antagonists of N-methyl-D-aspartate based on density functional theory with electronic and topological descriptors. Journal of Taibah University for Science, 2015, 9, 143-154.	1.1	31
68	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