Adnane Aouidate

List of Publications by Year
in descending order

24 papers	583 citations	623574 14 h-index	642610 23 g-index
24 all docs	24 docs citations	24 times ranked	604 citing authors

#	Article	IF	Citations
1	In silico molecular investigations of pyridine N-Oxide compounds as potential inhibitors of SARS-CoV-2: 3D QSAR, molecular docking modeling, and ADMET screening. Journal of Biomolecular Structure and Dynamics, 2022, 40, 143-153.	2.0	24
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	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
4	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
5	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
6	Theoretical modeling and experimental studies of Terebinth extracts as green corrosion inhibitor for iron in 3% NaCl medium. Journal of King Saud University - Science, 2020, 32, 2995-3004.	1.6	43
7	Synthesis, antibacterial evaluation, in silico ADMET and molecular docking studies of new N-acylhydrazone derivatives from acridone. Arabian Journal of Chemistry, 2020, 13, 6236-6245.	2.3	20
8	Discovering Anti-Cancer Drugs via Computational Methods. Frontiers in Pharmacology, 2020, 11, 733.	1.6	148
9	In Silico Exploration of Aryl Halides Analogues as CheckpointKinase 1 Inhibitors by Using 3D QSAR, Molecular Docking Study,and ADMET Screening. Advanced Pharmaceutical Bulletin, 2019, 9, 84-92.	0.6	17
10	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
11	Antibacterial study of 3-(2-amino-6-phenylpyrimidin-4-yl)-N-cyclopropyl-1-methyl-1H-indole-2-carboxamide derivatives: CoMFA, CoMSIA analyses, molecular docking and ADMET properties prediction. Journal of Molecular Structure, 2019, 1177, 275-285.	1.8	11
12	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
13	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
14	3D QSAR studies, molecular docking and ADMET evaluation, using thiazolidine derivatives as template to obtain new inhibitors of PIM1 kinase. Computational Biology and Chemistry, 2018, 74, 201-211.	1.1	15
15	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
16	Theoretical Study of Copper Acetonitrile Effects on Parr Functions Indices and Regioselectivity Using Density Functional Theory (DFT). Russian Journal of Physical Chemistry A, 2018, 92, 2464-2471.	0.1	3
17	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
18	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

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19	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
20	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
21	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
22	3D-QSAR modeling and molecular docking studies on a series of 2,5 disubstituted 1,3,4-oxadiazoles. Journal of Molecular Structure, 2017, 1145, 278-284.	1.8	22
23	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
24	Theoretical Study of 1,3-Dipolar Cycloadditions Regioselectivity of Benzyl Azide with Glycosyl-O Acetylene Using Density Functional Theory (DFT). Orbital, 2017, 9, .	0.1	0