

# Adnane Aouidate

## List of Publications by Year in descending order

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24  
papers

583  
citations

623574

14  
h-index

642610

23  
g-index

24  
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24  
docs citations

24  
times ranked

604  
citing authors

#	ARTICLE	IF	CITATIONS
1	Discovering Anti-Cancer Drugs via Computational Methods. <i>Frontiers in Pharmacology</i> , 2020, 11, 733.	1.6	148
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. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 4522-4535.	2.0	49
3	Theoretical modeling and experimental studies of Terebinth extracts as green corrosion inhibitor for iron in 3% NaCl medium. <i>Journal of King Saud University - Science</i> , 2020, 32, 2995-3004.	1.6	43
4	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
5	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
6	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
7	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
8	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
9	In silico molecular investigations of pyridine N-Oxide compounds as potential inhibitors of SARS-CoV-2: 3D QSAR, molecular docking modeling, and ADMET screening. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 143-153.	2.0	24
10	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
11	3D-QSAR modeling and molecular docking studies on a series of 2,5 disubstituted 1,3,4-oxadiazoles. <i>Journal of Molecular Structure</i> , 2017, 1145, 278-284.	1.8	22
12	Synthesis, antibacterial evaluation, in silico ADMET and molecular docking studies of new N-acylhydrazone derivatives from acridone. <i>Arabian Journal of Chemistry</i> , 2020, 13, 6236-6245.	2.3	20
13	In Silico Exploration of Aryl Halides Analogues as CheckpointKinase 1 Inhibitors by Using 3D QSAR, Molecular Docking Study, and ADMET Screening. <i>Advanced Pharmaceutical Bulletin</i> , 2019, 9, 84-92.	0.6	17
14	3D QSAR studies, molecular docking and ADMET evaluation, using thiazolidine derivatives as template to obtain new inhibitors of PIM1 kinase. <i>Computational Biology and Chemistry</i> , 2018, 74, 201-211.	1.1	15
15	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
16	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
17	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. <i>Journal of Molecular Structure</i> . 2019, 1177, 275-285.	1.8	11
18	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

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19	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
20	Structural basis of pyrazolopyrimidine derivatives as CAMKII $\beta$ kinase inhibitors: insights from 3D QSAR, docking studies and in silico ADMET evaluation. Chemical Papers, 2018, 72, 2833-2847.	1.0	4
21	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
22	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
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