Sorin Avram

List of Publications by Year
in descending order

31 papers	432 citations	840776 11 h-index	794594 19 g-index
31 all docs	31 docs citations	31 times ranked	630 citing authors

#	Article	IF	Citations
1	Large-scale comparison between the diffraction-component precision indexes favors Cruickshankâ€™s Rfree function. Journal of the Serbian Chemical Society, 2022, 87, 321-330.	0.8	0
2	Comprehensive investigation of selectivity landscape of glycogen synthase kinase-3 inhibitors. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2318-2337.	3.5	1
3	DrugCentral 2021 supports drug discovery and repositioning. Nucleic Acids Research, 2021, 49, D1160-D1169.	14.5	129
4	The B-factor index for the binding site (BFIbs) to prioritize crystal protein structures for docking. Structural Chemistry, 2021, 32, 1693-1699.	2.0	1
5	Novel drug targets in 2020. Nature Reviews Drug Discovery, 2021, 20, 333-333.	46.4	5
6	Structure- and ligand- based studies to gain insight into the pharmacological implications of histamine H3 receptor. Structural Chemistry, 2021, 32, 1141-1149.	2.0	2
7	Off-Patent Drug Repositioning. Journal of Chemical Information and Modeling, 2020, 60, 5746-5753.	5.4	14
8	Partial Least Squares Discriminant Analysis and 3D Similarity Perspective Applied to Analyze Comprehensively the Selectivity of Glycogen Synthase Kinase 3 Inhibitors. Molecular Informatics, 2020, 39, 1900142.	2.5	1
9	Novel drug targets in 2019. Nature Reviews Drug Discovery, 2020, 19, 300-300.	46.4	12
10	In silico studies on smoothened human receptor and its antagonists in search of anticancer effects. Journal of the Serbian Chemical Society, 2020, 85, 335-346.	0.8	0
11	Portraying the selectivity of GSK-3 inhibitors towards CDK-2 by 3D similarity and molecular docking. Structural Chemistry, 2019, 30, 911-923.	2.0	6
12	Modeling Kinase Inhibition Using Highly Confident Data Sets. Journal of Chemical Information and Modeling, 2018, 58, 957-967.	5.4	17
13	Enhancing Molecular Promiscuity Evaluation Through Assay Profiles. Pharmaceutical Research, 2018, 35, 240.	3.5	3
14	Design, Synthesis and Biological Activity Evaluation of S-Substituted 1H-5-Mercapto-1,2,4-Triazole Derivatives as Antiproliferative Agents in Colorectal Cancer. Frontiers in Chemistry, 2018, 6, 373.	3.6	20
15	Pharmacophore-based screening and drug repurposing exemplified on glycogen synthase kinase-3 inhibitors. Molecular Diversity, 2017, 21, 385-405.	3.9	17
16	Design, synthesis and pharmaco-toxicological assessment of 5-mercapto-1,2,4-triazole derivatives with antibacterial and antiproliferative activity. International Journal of Oncology, 2017, 50, 1175-1183.	3.3	24
17	Docking Study of 3-mercapto-1,2,4-triazole Derivatives as Inhibitors for VEGFR and EGFR. Revista De Chimie (discontinued), 2017, 68, 500-503.	0.4	4
18	Synthesis, Characterization and Antiproliferative Activity Assessment of a Novel 1H-5-mercapto-1,2,4 Triazole Derivative. Revista De Chimie (discontinued), 2017, 68, 745-747.	0.4	4

#	Article	IF	Citations
19	Predictive Models for Fast and Effective Profiling of Kinase Inhibitors. Journal of Chemical Information and Modeling, 2016, 56, 895-905.	5.4	23
20	Quantitative estimation of pesticide-likeness for agrochemical discovery. Journal of Cheminformatics, 2014, 6, 42.	6.1	61
21	PLS and shape-based similarity analysis of maleimides â€“ GSK-3 inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2014, 29, 599-610.	5.2	10
22	Exploring the biological promiscuity of high-throughput screening hits through DFT calculations. Bioorganic and Medicinal Chemistry, 2014, 22, 2461-2468.	3.0	13
23	ColBioS-FlavRC: A Collection of Bioselective Flavonoids and Related Compounds Filtered from High-Throughput Screening Outcomes. Journal of Chemical Information and Modeling, 2014, 54, 2360-2370.	5.4	14
24	Challenges in docking 2â€²-hydroxy and 2â€²,4â€²-dihydroxychalcones into the binding site of ALR2. Medicinal Chemistry Research, 2013, 22, 3589-3605.	2.4	5
25	Implementation of PLS discriminant analysis to rank indirubin derivatives against decoys. Open Chemistry, 2013, 11, 1644-1656.	1.9	0
26	QSAR study and molecular docking on indirubin inhibitors of Glycogen Synthase Kinase-3. Open Chemistry, 2013, 11, 63-77.	1.9	9
27	Retrospective group fusion similarity search based on eROCE evaluation metric. Bioorganic and Medicinal Chemistry, 2013, 21, 1268-1278.	3.0	12
28	Modeling of 2-Pyridin-3-yl-Benzo[d][1,3]Oxazin-4-one Derivatives by Several Conformational Searching Tools and Molecular Docking. Current Pharmaceutical Design, 2013, 19, 2194-2203.	1.9	4
29	In silico classification and virtual screening of maleimide derivatives using projection to latent structures discriminant analysis (PLS-DA) and hybrid docking. Monatshefte FÃ¼r Chemie, 2012, 143, 1559-1573.	1.8	4
30	PLS-DA - Docking Optimized Combined Energetic Terms (PLSDA-DOCET) Protocol: A Brief Evaluation. Journal of Chemical Information and Modeling, 2011, 51, 3169-3179.	5.4	17
31	MTD-PLS and docking study for a series of substituted 2-phenylindole derivatives with oestrogenic activity. Chemical Papers, 2011, 65, .	2.2	0