

Lead- and drug-like compounds: the rule-of-five revolution

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Structure-activity relationships of 1-alkyl-5-(3,4-dichlorophenyl)-5-[2-[3-(substituted)-1-azetidyl]-ethyl]-2-piperidones. Part 2: Improving oral absorption. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 3957-3961.	1.0	9
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1293	Discovery of novel aminopiperidinyl amide CXCR4 modulators through virtual screening and rational drug design. <i>European Journal of Medicinal Chemistry</i> , 2020, 201, 112479.	2.6	9
1294	Mitigation of heterocyclic aromatic amines in cooked meat. Part I: Informed selection of antioxidants based on molecular modeling. <i>Food Chemistry</i> , 2020, 331, 127264.	4.2	16
1295	Synthesis, Characterization, Biological Screening, ADME and Molecular Docking Studies of 2-Phenyl Quinoline-4-Carboxamide Derivatives. <i>Asian Journal of Chemistry</i> , 2020, 32, 1151-1157.	0.1	3
1296	Characterization of Polymeric Syringes Used for Intravitreal Injection. <i>Journal of Pharmaceutical Sciences</i> , 2020, 109, 2812-2818.	1.6	4
1297	Synthesis and Biological Activity of Ethyl 2-[8-Arylmethylidenehydrazino-3-Methyl-7-(1-Oxothietan-3-YL)Xanth-1-YL]Acetates. <i>Pharmaceutical Chemistry Journal</i> , 2020, 54, 213-219.	0.3	3
1298	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
1299	<i>Thalictrum foliolosum</i> DC: An unexplored medicinal herb from north western Himalayas with potential against fungal pathogens and scavenger of reactive oxygen species. <i>Biocatalysis and Agricultural Biotechnology</i> , 2020, 26, 101621.	1.5	11
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1301	Computational methods and tools for sustainable and green approaches in drug discovery. , 2020, , 965-988.		3
1302	Targeting FTO Suppresses Cancer Stem Cell Maintenance and Immune Evasion. <i>Cancer Cell</i> , 2020, 38, 79-96.e11.	7.7	389
1303	Synthesis, characterization, electrochemistry, biological and molecular docking studies of the novel Co(II), Ni(II) and Cu(II) complexes derived from methanethiol bridged (2-((1H-benzo[d]imidazol-2-yl)methylthio)-1H-benzo[d]imidazol-6-yl)(phenyl)methanone. <i>Journal of Molecular Structure</i> , 2020, 1220, 128586.	1.8	9
1304	Quantitative structure-activity relationship methods in the discovery and development of antibacterials. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1472.	6.2	9
1305	Reveals of New Candidate Active Components in <i>Hemerocallis Radix</i> and Its Anti-Depression Action of Mechanism Based on Network Pharmacology Approach. <i>International Journal of Molecular Sciences</i> , 2020, 21, 1868.	1.8	25
1306	Translating traditional herbal formulas into modern drugs: a network-based analysis of Xiaoyao decoction. <i>Chinese Medicine</i> , 2020, 15, 25.	1.6	16
1307	Cheminformatics approaches to assess chemical diversity and complexity of small molecules. , 2020, , 83-102.		8
1308	Synthesis and Antiproliferative Screening Of Novel Analogs of Regioselectively Demethylated Colchicine and Thiocolchicine. <i>Molecules</i> , 2020, 25, 1180.	1.7	9
1309	Exploring Quinazolinones as Anticonvulsants by Molecular Fragmentation Approach: Structural Optimization, Synthesis and Pharmacological Evaluation Studies. <i>ChemistrySelect</i> , 2020, 5, 2902-2912.	0.7	9

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1314	Novel Acetylcholinesterase Inhibitors Identified from ZINC Database Using Dockingâ€”Based Virtual Screening for Alzheimer's Disease.. <i>ChemistrySelect</i> , 2020, 5, 3593-3599.	0.7	6
1315	How We Think about Targeting RNA with Small Molecules. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 8880-8900.	2.9	109
1316	Synthesis, <i>in-vitro</i> antibacterial and anticancer screening of novel nicotinonitrile-coumarin hybrids utilizing piperazine citrate. <i>Synthetic Communications</i> , 2020, 50, 1468-1485.	1.1	34
1317	Computational and in vitro Pharmacodynamics Characterization of 1A-116 Rac1 Inhibitor: Relevance of Trp56 in Its Biological Activity. <i>Frontiers in Cell and Developmental Biology</i> , 2020, 8, 240.	1.8	7
1318	Photocatalytic [2 + 2] Cycloaddition in DNA-Encoded Chemistry. <i>Organic Letters</i> , 2020, 22, 2908-2913.	2.4	51
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1322	Synthesis and docking studies of three new diaminochromenes as potential leads for anticancer drugs. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 39, 1-9.	2.0	0
1323	Preliminary Investigation of the Antibacterial Activity of Antitumor Drug 3-Amino-1,2,4-Benzotriazine-1,4-Dioxide (Tirapazamine) and its Derivatives. <i>Applied Sciences (Switzerland)</i> , 2020, 10, 4062.	1.3	3
1324	Benchmarking Data Sets from PubChem BioAssay Data: Current Scenario and Room for Improvement. <i>International Journal of Molecular Sciences</i> , 2020, 21, 4380.	1.8	8
1325	Chemical interaction analysis of L-Theanine compounds from <i>Camellia sinensis</i> L. with kainate glutamate receptors and their toxicity effect as anti autism candidates based on in silico. <i>AIP Conference Proceedings</i> , 2020, . .	0.3	2
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1339	Testicular Caspase-3 and β -Catenin Regulators Predicted via Comparative Metabolomics and Docking Studies. <i>Metabolites</i> , 2020, 10, 31.	1.3	14
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1341	Large-Scale Virtual Screening Against the MET Kinase Domain Identifies a New Putative Inhibitor Type. <i>Molecules</i> , 2020, 25, 938.	1.7	7
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1343	A deep learning approach for the blind logP prediction in SAMPL6 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 535-542.	1.3	19
1344	Exploring the ethnomycological potential of <i>Lentinus squarrosulus</i> Mont. through GC-MS and chemoinformatics tools. <i>Mycology</i> , 2020, 11, 78-89.	2.0	7
1345	An efficient and targeted synthetic approach towards new highly substituted 6-amino-pyrazolo[1,5- <i>a</i>]pyrimidines with β -glucosidase inhibitory activity. <i>Scientific Reports</i> , 2020, 10, 2595.	1.6	27

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1348	Wavefunction analysis, charge transfer and molecular docking studies on famciclovir and entecavir: Potential anti-viral drugs. <i>Chemical Data Collections</i> , 2020, 26, 100353.	1.1	6
1349	Novel androgen receptor antagonist identified by structure-based virtual screening, structural optimization, and biological evaluation. <i>European Journal of Medicinal Chemistry</i> , 2020, 192, 112156.	2.6	15
1350	Photochemical Internalization for Intracellular Drug Delivery. From Basic Mechanisms to Clinical Research. <i>Journal of Clinical Medicine</i> , 2020, 9, 528.	1.0	60
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1354	Salicornolides A-C from <i>Gracilaria salicornia</i> attenuate pro-inflammatory 5-lipoxygenase: Prospective natural anti-inflammatory leads. <i>Phytochemistry</i> , 2020, 172, 112259.	1.4	10
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1359	Synthesis and Molecular Modelling Studies of Coumarin and 1-Aza-Coumarin Linked Miconazole Analogues and Their Antimicrobial Properties. <i>ChemistrySelect</i> , 2020, 5, 1322-1330.	0.7	8
1361	Synthesis, docking and in vitro evaluation of γ -proline derived 1,3-diketones possessing anti-cancer and anti-inflammatory activities. <i>Journal of Molecular Structure</i> , 2020, 1206, 127754.	1.8	11
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1367	3D-QSAR and Pharmacophore modeling of 3,5-disubstituted indole derivatives as Pim kinase inhibitors. <i>Structural Chemistry</i> , 2020, 31, 1675-1690.	1.0	17
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1384	Drug repurposing for coronavirus (COVID-19): <i>in silico</i> screening of known drugs against coronavirus 3CL hydrolase and protease enzymes. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 2980-2992.	2.0	284
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1572	Stereo- and regiodefined DNA-encoded chemical libraries enable efficient tumour-targeting applications. <i>Nature Chemistry</i> , 2021, 13, 540-548.	6.6	42
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1585	Antidepressant activity of rose oxide essential oil: possible involvement of serotonergic transmission. <i>Heliyon</i> , 2021, 7, e06620.	1.4	10
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1923	Skp1 in lung cancer: clinical significance and therapeutic efficacy of its small molecule inhibitors. <i>Oncotarget</i> , 2015, 6, 34953-34967.	0.8	53
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1929	Chemical Structure Similarity Search for Ligand-based Virtual Screening: Methods and Computational Resources. <i>Current Drug Targets</i> , 2016, 17, 1580-1585.	1.0	40
1930	Screening of Anti-mycobacterial Phytochemical Compounds for Potential Inhibitors against <i>Mycobacterium Tuberculosis</i> Isocitrate Lyase. <i>Current Topics in Medicinal Chemistry</i> , 2019, 19, 600-608.	1.0	8
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1992	Insights into Weak and Covalent Interactions, Reactivity sites and Pharmacokinetic Studies of 4-Dimethylaminopyridinium Salicylate Monohydrate using Quantum Chemical Computation method. <i>Computational and Theoretical Chemistry</i> , 2021, 1206, 113483.	1.1	8
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2002	Synthesis, Biological, and Molecular Docking Studies on 4,5,6,7-Tetrahydrobenzo[<i>b</i>]thiophene Derivatives and Their Nanoparticles Targeting Colorectal Cancer. <i>ACS Omega</i> , 2021, 6, 28992-29008.	1.6	5
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