

ADMETlab 2.0: an integrated online platform for accurate prediction of ADMET properties

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Citation Report

#	ARTICLE	IF	CITATIONS
1	GC-MS analysis and in silico assessment of constituents of <i>Psidium guajava</i> leaf extract against DNA gyrase of <i>Salmonella enterica</i> serovar Typhi. <i>Informatics in Medicine Unlocked</i> , 2021, 26, 100722.	1.9	7
2	Identification of Kaurane-Type Diterpenes as Inhibitors of <i>Leishmania</i> Pteridine Reductase I. <i>Molecules</i> , 2021, 26, 3076.	1.7	11
3	Towards the sustainable discovery and development of new antibiotics. <i>Nature Reviews Chemistry</i> , 2021, 5, 726-749.	13.8	439
4	Learning to SMILES: BAN-based strategies to improve latent representation learning from molecules. <i>Briefings in Bioinformatics</i> , 2021, 22, .	3.2	25
5	Discovery of novel inhibitors of SARS-CoV-2 main protease. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 12526-12534.	2.0	2
6	FP-ADMET: a compendium of fingerprint-based ADMET prediction models. <i>Journal of Cheminformatics</i> , 2021, 13, 75.	2.8	39
7	<i>In silico</i> and <i>in vitro</i> evaluation of efflux pumps inhibition of $\Delta^{\pm,12}$ -amyrin. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 12785-12799.	2.0	12
9	Screening of <i>Azadirachta indica</i> phytoconstituents as GSK-3 β inhibitor and its implication in neuroblastoma: molecular docking, molecular dynamics, MM-PBSA binding energy, and in-vitro study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 12827-12840.	2.0	10
10	Anticancer agents based on Plastoquinone analogs with N-phenylpiperazine: Structure-activity relationship and mechanism of action in breast cancer cells. <i>Chemico-Biological Interactions</i> , 2021, 349, 109673.	1.7	11
11	Computational strategies towards developing novel SARS-CoV-2 Mpro inhibitors against COVID-19. <i>Journal of Molecular Structure</i> , 2022, 1247, 131378.	1.8	11
12	'In silico' toxicology methods in drug safety assessment. <i>Arhiv Za Farmaciju</i> , 2021, 71, 257-278.	0.2	0
13	DDInter: an online drug-drug interaction database towards improving clinical decision-making and patient safety. <i>Nucleic Acids Research</i> , 2022, 50, D1200-D1207.	6.5	37
14	Novel Hydroxytyrosol-Donepezil Hybrids as Potential Antioxidant and Neuroprotective Agents. <i>Frontiers in Chemistry</i> , 2021, 9, 741444.	1.8	15
15	Virtual screening using docking and molecular dynamics of cannabinoid analogs against CB1 and CB2 receptors. <i>Computational Biology and Chemistry</i> , 2021, 95, 107590.	1.1	14
16	Extracting Predictive Representations from Hundreds of Millions of Molecules. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 10793-10801.	2.1	28
17	Proteome-Informed Machine Learning Studies of Cocaine Addiction. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 11122-11134.	2.1	8
18	Computational design of new tacrine analogs: an in silico prediction of their cholinesterase inhibitory, antioxidant, and hepatotoxic activities. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-15.	2.0	2
19	PPAR β , adiponectin, and GLUT4 overexpression induced by moronic acid methyl ester influenced glucose and triglyceride levels of experimental diabetic mice. <i>Canadian Journal of Physiology and Pharmacology</i> , 2022, 100, 295-305.	0.7	2

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20	Semi-automated workflow for molecular pair analysis and QSAR-assisted transformation space expansion. <i>Journal of Cheminformatics</i> , 2021, 13, 86.	2.8	3
21	KK-DBP: A Multi-Feature Fusion Method for DNA-Binding Protein Identification Based on Random Forest. <i>Frontiers in Genetics</i> , 2021, 12, 811158.	1.1	7
22	Theoretically exploring selective-binding mechanisms of BRD4 through integrative computational approaches. <i>SAR and QSAR in Environmental Research</i> , 2021, 32, 1-27.	1.0	4
23	Structural and spectroscopic analysis, ADMET study, and anxiolytic-like effect in adult zebrafish (<i>Danio rerio</i>) of 4-[(1E,2E)-1-(2-(2,4-dinitrophenyl)hydrazono-3-(4-methoxyphenyl)allyl)aniline. <i>Journal of Molecular Structure</i> , 2022, 1251, 132064.	1.8	3
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27	In Silico Studies of Tumor Targeted Peptide-Conjugated Natural Products for Targeting Over-Expressed Receptors in Breast Cancer Cells Using Molecular Docking, Molecular Dynamics and MMGBSA Calculations. <i>Applied Sciences (Switzerland)</i> , 2022, 12, 515.	1.3	6
28	In Silico Screening of Potential Phytochemicals from Several Herbs against SARS-CoV-2 Indian Delta Variant B.1.617.2 to Inhibit the Spike Glycoprotein Trimer. <i>Applied Sciences (Switzerland)</i> , 2022, 12, 665.	1.3	8
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31	Development of New Antimicrobial Oleanonic Acid Polyamine Conjugates. <i>Antibiotics</i> , 2022, 11, 94.	1.5	8
32	Design, Synthesis and Evaluation of Novel (E)-N'-((1-(4-chlorobenzyl)-1H-indol-3-yl)methylene)-2-(4-oxoquinazolin-3(4H)-yl)acetohydrazides as Antitumor Agents. <i>Anti-Cancer Agents in Medicinal Chemistry</i> , 2022, 22, .	0.9	0
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34	Machine learning-driven identification of drugs inhibiting cytochrome P450 2C9. <i>PLoS Computational Biology</i> , 2022, 18, e1009820.	1.5	11
35	<i>Ruellia prostrata</i> Poir. activity evaluated by phytoconstituents, antioxidant, anti-inflammatory, antibacterial activity, and in silico molecular functions. <i>Journal of Saudi Chemical Society</i> , 2022, 26, 101401.	2.4	11
36	Synthesis, In Vitro, In Vivo and In Silico Antidiabetic Bioassays of 4-Nitro(thio)phenoxyisobutyric Acids Acting as Unexpected PPAR γ Modulators: An In Combo Study. <i>Pharmaceuticals</i> , 2022, 15, 102.	1.7	4
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39	Multitarget Hybrid Fasudil Derivatives as a New Approach to the Potential Treatment of Amyotrophic Lateral Sclerosis. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 1867-1882.	2.9	11
40	Design, synthesis, antimicrobial evaluations and in silico studies of novel pyrazol-5(4H)-one and 1H-pyrazol-5-ol derivatives. <i>Arabian Journal of Chemistry</i> , 2022, 15, 103682.	2.3	7
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53	Computational prediction of drug phenotypic effects based on substructure-phenotype associations. <i>IEEE/ACM Transactions on Computational Biology and Bioinformatics</i> , 2022, PP, 1-1.	1.9	0
54	Interpretable-ADMET: a web service for ADMET prediction and optimization based on deep neural representation. <i>Bioinformatics</i> , 2022, 38, 2863-2871.	1.8	21
55	Knowledge-based BERT: a method to extract molecular features like computational chemists. <i>Briefings in Bioinformatics</i> , 2022, 23, .	3.2	24

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61	Synthesis and in silico anti-metastatic evaluation of carvacrol derivative, 2-hydroxy-6-isopropyl-3-methylbenzaldehyde. <i>Materials Today: Proceedings</i> , 2022, 57, 739-747.	0.9	1
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71	Machine Learning Analysis of Cocaine Addiction Informed by DAT, SERT, and NET-Based Interactome Networks. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2703-2719.	2.3	8
72	IP-Se-06, a Selenylated Imidazo[1,2-a]pyridine, Modulates Intracellular Redox State and Causes Akt/mTOR/HIF-1 α and MAPK Signaling Inhibition, Promoting Antiproliferative Effect and Apoptosis in Glioblastoma Cells. <i>Oxidative Medicine and Cellular Longevity</i> , 2022, 2022, 1-18.	1.9	15
73	An efficient curriculum learning-based strategy for molecular graph learning. <i>Briefings in Bioinformatics</i> , 2022, 23, .	3.2	7

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75	In Silico Identification and Mechanism Exploration of Active Ingredients against Stroke from An-Gong-Niu-Huang-Wan (AGNHW) Formula. <i>Oxidative Medicine and Cellular Longevity</i> , 2022, 2022, 1-16.	1.9	3
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79	Synthesis and biological evaluation of cytotoxic activity of novel podophyllotoxin derivatives incorporating piperazinyl-cinnamic amide moieties. <i>Bioorganic Chemistry</i> , 2022, 123, 105761.	2.0	11
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88	Identification of Bioactive Components of <i>Stephania epigaea</i> Lo and Their Potential Therapeutic Targets by UPLC-MS/MS and Network Pharmacology. <i>Evidence-based Complementary and Alternative Medicine</i> , 2022, 2022, 1-11.	0.5	1
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93	Synthesis, spectral analysis, DFT calculations, biological potential and molecular docking studies of indole appended pyrazolo-triazine. <i>Molecular Diversity</i> , 2023, 27, 679-693.	2.1	14
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96	Natural Compound ZINC12899676 Reduces Porcine Epidemic Diarrhea Virus Replication by Inhibiting the Viral NTPase Activity. <i>Frontiers in Pharmacology</i> , 2022, 13, .	1.6	2
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98	Investigation of antidiabetic properties of shikonin by targeting aldose reductase enzyme: In silico and in vitro studies. <i>Biomedicine and Pharmacotherapy</i> , 2022, 150, 112985.	2.5	7
99	Fatty acid composition, acute toxicity and anti-inflammatory activity of the n-hexane extract from <i>Ranunculus macrophyllus</i> Desf. roots. <i>South African Journal of Botany</i> , 2022, 148, 315-325.	1.2	6
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