Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings

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602	Novel N-(4-thiocyanatophenyl)-1H-1,2,3-triazole-4-carboxamides exhibit selective cytotoxic activity at nanomolar doses towards human leukemic T-cells. **2022**, 241, 114633	1
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520	Ethyl 5-Oxo-5-(((12-oxoindolo[2,1-b]quinazolin-6(12H)-ylidene)amino)oxy)pentanoate. **2022**, 2022, M1451	0
519	Network Analysis of the Herb–Drug Interactions of Citrus Herbs Inspired by the "Grapefruit Juice Effect"	1
518	Peptides as Pharmacological Carriers to the Brain: Promises, Shortcomings and Challenges.	1

517	GC-MS Screening of Adiantum lunulatum Burm. F Phytochemicals and interaction with COX-2, TRPV1, and TRPC3 proteins-bioinformatics approach.. **2022**, 18,	0
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505	A New Formulation for the Concerted Alchemical Calculation of van der Waals and Coulomb Components of Solvation Free Energies.	0
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483	A fast-killing tyrosine amide ((S)-SW228703) with blood and liver-stage antimalarial activity associated with the Cyclic Amine Resistance Locus (PfCARL).	0
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481	Polymyxin B Activity Rescue by (1)-Camphene-Based Thiosemicarbazide Against Carbapenem-Resistant Enterobacterales. **2022**, 28, 962-971	0
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471	CADMA-Chem: A Computational Protocol Based on Chemical Properties Aimed to Design Multifunctional Antioxidants. **2022**, 23, 13246	2
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462	Drug candidates and potential targets of Curculigo spp. compounds for treating diabetes mellitus based on network pharmacology, molecular docking and molecular dynamics simulation. 1-17	0
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458	Network pharmacology analysis reveals neuroprotective effects of the Qin-Zhi-Zhu-Dan Formula in Alzheimer□s disease. 16,	0
457	1,2,3-Triazole Linked Chalcone-Morpholine Hybrids: Synthesis, In Vitro Antibacterial Evaluation and In Silico ADMET Predictions. 1-17	0
456	Toward Realistic Dosimetry In Vitro: Determining Effective Concentrations of Test Substances in Cell Culture and Their Prediction by an In Silico Mass Balance Model.	0
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444	Structural characterization, molecular docking assessment, drug-likeness study and DFT investigation of 2-(2-{1,2-dibromo-2-[3-(4-chloro-phenyl)-[1,2,4]oxadiazol-5-yl]-2-fluoro-ethyl1}-phenyl)-methyl 3-methoxy-acrylic ester. **2022**, 99, 100745	0
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435	Selective Separation and Preconcentration of Caffeine from Natural and Pharmaceutical Products using New Polyurethane Foams. 58,	0
434	From Anti-Parkinson's Drug Rasagiline to Novel Multitarget Iron Chelators with Acetylcholinesterase and Monoamine Oxidase Inhibitory and Neuroprotective Properties for Alzheimer's Disease. **2022**, 3167-3192	0
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430	Practical approach to N-benzyl derivatives of 2-amino-8-methoxy-4H-chromene-3-carbonitrile by reductive amination: Exploration of their effects against protein kinases and in silico ADME profiling. **2023**, 1274, 134319	0
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428	Dual Targeting of MDM4 and FTH1 by MMRi71 for Induced Protein Degradation and p53-Independent Apoptosis in Leukemia Cells. **2022**, 27, 7665	0

427	The use of machine learning modeling, virtual screening, molecular docking, and molecular dynamics simulations to identify potential VEGFR2 kinase inhibitors. **2022**, 12,	1
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422	Vetinformatics from functional genomics to drug discovery: Insights into decoding complex molecular mechanisms of livestock systems in veterinary science. 9,	0
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416	Virtual Screening and In Vitro Experiments Highlight Cannabidiol as a Drug-like Phosphodiesterase 9 Inhibitor.	1
415	Novel 1,2,4-triazoles derived from Ibuprofen: synthesis and in vitro evaluation of their mPGES-1 inhibitory and antiproliferative activity.	0
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18	Compounds Interacting with Cholecystokinin as Potential Drugs Against Excessive Weight Gain and Obesity. **2023**, 8,	0
17	MOLECULAR HYBRID OF 1,2,3-TRIAZOLE AND SCHIFF BASE AS POTENTIAL ANTIBACTERIAL AGENTS: DFT, MOLECULAR DOCKING AND ADME STUDIES. **2023**, 135617	0
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