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

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548	Heterosynthons, Solid Form Design and Enhanced Drug Bioavailability.	1

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538	Design, synthesis and biological evaluation of (Quinazoline 4-yloxy)acetamide and (4-oxoquinazoline-3(4H)-yl)acetamide derivatives as inhibitors of Mycobacterium tuberculosis bd oxidase. **2022**, 242, 114639	0
537	In silico ADMET, docking, anti-proliferative and antimicrobial evaluations of ethanolic extract of Euphorbia dendroides L.. **2022**, 150, 607-620	1
536	Syntheses and studies of deuterated Imdiazo[1,2-a]pyridine-3-carboxamides with potent anti-tuberculosis activity and improved metabolic properties. **2022**, 128, 106074	0
535	Design and synthesis of thiophenone and furanthione butenolide bioisosteres with inhibitory activity towards acetylcholinesterase. **2022**, 1269, 133831	
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525	Molecular docking studies on the binding interaction and stability of ovalbumin with an intramolecular charge transfer dye 4-dicyanomethylene-2,6-dimethyl-4H-pyran in the presence of an antibiotic: Tetracycline. **2022**, 99, 100681	2
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518	Immunomodulatory efficacy of Cousinia thomsonii C.B. Clarke in ameliorating inflammatory cascade expressions. **2023**, 300, 115727	0
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500	Computer-Aided Drug Design of Plant-Based Compounds. **2022**, 320-345	0
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490	In Vitro Antimicrobial Screening of Benzoylthioureas: Synthesis, Antibacterial Activity toward Streptococcus agalactiae and Molecular Docking Study. **2022**, 7,	0
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471	Comparative analysis of phytochemical composition and anti-oxidant and anti-inflammatory benefits of Eruca sativa grown at high altitude than at lower altitude.	0
470	Nonacidic thiophene-based derivatives as potential analgesic and design, synthesis, biological evaluation, and metabolic stability study.	0
469	Comparative Study of Drug Efficiency of Semecarpus anacardium and Tridax procumbens Against Zika Virus. **2023**, 183-202	0
468	Virtual screening of flavonoids from Chamaecrista genus: ADME and pharmacokinetic properties, interactions of flavonoidDNA complex by molecular docking and molecular dynamics. 1-9	0
467	In Silico Prediction of Anti-Infective and Cell-Penetrating Peptides from Thalassophryne nattereri Natterin Toxins. **2022**, 15, 1141	0
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460	A Computational Study of Carbazole Alkaloids from Murraya koenigii as Potential SARS-CoV-2 Main Protease Inhibitors.	1
459	The druggable genome: Twenty years later. 2,	0
458	Synthesis, cytotoxic evaluation and ct-DNA binding of series of 1,4-disubstituted anthraquinone-sulfonamide conjugates. **2022**, 134,	0

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454	Phthalimide-tethered imidazolium salts: Synthesis, characterization, enzyme inhibitory properties, and in silico studies.	0
453	Design, Synthesis and biological evaluation of novel benzopyran derivatives as potential □amylase inhibitors: An Investigation by Experimental and Computational Studies. **2022**, 134227	0
452	Synthesis, Antibacterial, and Antioxidant Activities of Thiazolyl-Pyrazoline Schiff Base Hybrids: A Combined Experimental and Computational Study. **2022**, 2022, 1-19	0
451	Flavonoids as promising anticancer agents: an in silico investigation of ADMET, binding affinity by molecular docking and molecular dynamics simulations. 1-12	0
450	Dimensionally Reduced Machine Learning Model for Predicting Single Component Octanol-Water Partition Coefficients.	0
449	In silico approach identified benzoylguanidines as SARS-CoV-2 main protease (Mpro) potential inhibitors. 1-14	1
448	LC□MS/MS Phytochemical Profiling, Antioxidant Activity, and Cytotoxicity of the Ethanolic Extract of Atriplex halimus L. against Breast Cancer Cell Lines: Computational Studies and Experimental Validation. **2022**, 15, 1156	2
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446	Overcoming the blood□brain barrier for the therapy of malignant brain tumor: current status and prospects of drug delivery approaches. **2022**, 20,	4
445	Synthesis and Biological Activity Evaluation of Benzothiazole-isoquinoline Derivatives.	0
444	Metabolite profiling, In-vitro and insilico assessment of antibacterial and anticancer activities of Alternaria alternata endophytic in Jatropha heynei.	0
443	Homology Modeling, Molecular Docking, Molecular Dynamic Simulation, and Drug-Likeness of the Modified Alpha-Mangostin against the □Tubulin Protein of Acanthamoeba Keratitis. **2022**, 27, 6338	0
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439	Implications of Coexistent Halogen and Hydrogen Bonds in Amorphous Solid Dispersions on Drug Solubility, Miscibility, and Mobility.	0
438	Integrating Pharmacological and Computational Approaches for the Phytochemical Analysis of Syzygium cumini and Its Anti-Diabetic Potential. **2022**, 27, 5734	0
437	Identification of Concomitant Inhibitors against Glutamine Synthetase and Isocitrate Lyase in Mycobacterium tuberculosis from Natural Sources. **2022**, 2022, 1-14	0
436	Protective Mechanisms of Nootropic Herb Shankhpushpi (Convolvulus pluricaulis) against Dementia: Network Pharmacology and Computational Approach. **2022**, 2022, 1-18	0
435	Integrated Spectroscopic, Bio-active Prediction and Analytics of Isoquinoline Derivative for Breast Cancer Mitigation.	4
434	Biological Activity of Two Anticancer Pt Complexes with a Cyclohexylglycine Ligand against a Colon Cancer Cell Line: Theoretical and Experimental Study.	1
433	Predictive validity in drug discovery: what it is, why it matters and how to improve it.	4
432	Synthesis, Structural Characterization, X-ray, Hirshfeld Surfaces, DFT calculations, In Silico ADME Approach and a Molecular Docking Study of a New Nickel(II) Complex. **2022**, 7,	0
431	Design and Synthesis of Fsp3-enriched Spirocyclic-Based Biological Screening Compound Arrays via DOS strategies and their NNMT Inhibition Profiling..	0
430	Pyridine-N-Oxide Alkaloids from Allium stipitatum and Their Synthetic Disulfide Analogs as Potential Drug Candidates against Mycobacterium tuberculosis: A Molecular Docking, QSBAR, and ADMET Prediction Approach. **2022**, 2022, 1-14	0
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428	Targeting human thymidylate synthase: Ensemble-based virtual screening for drug repositioning and the role of water. **2022**, 108348	0
427	In silico and biological exploration of greenly synthesized curcumin-incorporated isoniazid Schiff base and its ruthenium complexes.	0
426	Time Matters In vitro Cellular Disposition Kinetics Help Rationalizing Cellular Potency Disconnects. 1-39	0
425	Multi-target direct-acting SARS-CoV-2 antivirals against the nucleotide-binding pockets of virus-specific proteins. **2022**,	0
424	DFT-based computations on some structurally related N-substituted piperazines. **2022**, 100766	1
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421	Structure based design and synthesis of 3-(7-nitro-3-oxo-3,4-dihydroquinoxalin-2-yl)propanehydrazide derivatives as novel bacterial DNA-gyrase inhibitors: In-vitro, In-vivo, In-silico and SAR studies. **2022**, 129, 106186	1
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418	Expanding the scope of novel 1,2,3-triazole derivatives as new antiparasitic drug candidates.	0
417	Effect of substituents and chain length in amino-1,4-naphthoquinones on glutathione-S-transferase inhibition: molecular docking and electrochemical perspectives: a structure□activity study.	0
416	Quaternary Ru(II) Complexes of Terpyridines, Saccharin and 1, 2-Azoles: Effect of Substituents on Molecular Structure, Speciation, Photoactivity, and Photocytotoxicity.	0
415	Reinvigorate the synthesis, spectroscopic findings, SEM morphology investigation, and antimicrobial silhouette of contemporary Salen ligands: A comprehensive DFT landscape. **2022**, 4, 100574	0
414	In vitro studies on the selective cytotoxic effect of luminescent Ru(ii)-p-cymene complexes of imidazo-pyridine and imidazo quinoline ligands.	0
413	In-silico investigations on the anticancer activity of selected 2-aryloxazoline derivatives against breast cancer. 1-10	0
412	Carica papaya Reduces Muscle Insulin Resistance via IR/GLUT4 Mediated Signaling Mechanisms in High Fat Diet and Streptozotocin-Induced Type-2 Diabetic Rats. **2022**, 11, 2081	3
411	Antibacterial and Antioxidant Activities, in silico Molecular Docking, ADMET and DFT Analysis of Compounds from Roots of Cyphostemma cyphopetalum. Volume 15, 79-97	0
410	Antitumor activity against human promyelocytic leukemia and in silico studies of some benzoxazines. 1-16	0
409	Discovery of putative inhibitors against main drivers of SARS-CoV-2 infection: Insight from quantum mechanical evaluation and molecular modeling. 10,	0
408	Synthesis, Anticancer Evaluation and Pharmacokinetic Studies of Quinoline-Triazole Hybrid Derivatives. **2022**, 7,	0
407	Structure-Based Virtual Screening and De Novo Design to Identify Submicromolar Inhibitors of G2019S Mutant of Leucine-Rich Repeat Kinase 2. **2022**, 23, 12825	1
406	Predicting FDA approvability of small-molecule drugs.	0
405	Acetylphenyl-Substituted Imidazolium Salts: Synthesis, Characterization, in silico Studies and Inhibitory Properties against Some Metabolic Enzymes.	0
404	The Pharmacological Mechanism of Curcumin against Drug Resistance in Non-Small Cell Lung Cancer: Findings of Network Pharmacology and Bioinformatics Analysis. **2022**, 2022, 1-19	0

403	Non-specific binding of compounds in in vitro metabolism assays: A comparison of microsomal and hepatocyte binding in different species and an assessment of the accuracy of prediction models.. 1-47	0
402	Synthesizing, Studying Molecular Docking, Characterizing, and Preliminary Evaluating Anti-Bacterial Effects of Derivatives of Serotonin Contain Imidazolidine Ring. **2022**, 22, 1-16	0
401	Novel Unsymmetric 3,5-Bis(benzylidene)-4-piperidones That Display Tumor-Selective Toxicity. **2022**, 27, 6718	0
400	Psammaplysins: Insights from Natural Sources, Structural Variations, and Pharmacological Properties. **2022**, 20, 663	0
399	Screening of potential antiplasmodial agents targeting cysteine protease-Falcipain 2: a computational pipeline. 1-44	0
398	A Computational QSAR, Molecular Docking and In Vitro Cytotoxicity Study of Novel Thiouracil-Based Drugs with Anticancer Activity against Human-DNA Topoisomerase II. **2022**, 23, 11799	2
397	The Time and Place for Nature in Drug Discovery.	3
396	The computationally predicted drug-likeness, pharmacokinetics properties, medicinal chemistry parameters, and toxicity properties of Cucurbita maxima compounds.. 11, 1234	0
395	An open-source molecular builder and free energy preparation workflow. **2022**, 5,	0
394	Study of Biological Activities and ADMET-Related Properties of Salicylanilide-Based Peptidomimetics. **2022**, 23, 11648	1
393	Natural Phytocompounds from Common Indian Spices for Identification of Three Potential Inhibitors of Breast Cancer: A Molecular Modelling Approach. **2022**, 27, 6590	1
392	Going Viral: An Investigation into the Chameleonic Behavior or Antiviral Compounds.	0
391	Repurposing of Drugs Against Mutated Strain of Eurasian Avian Like H1N1 (EA H1N1) Swine Flu Virus, Genotype 4(G4) Virus.	0
390	Hydrogen-Bond Donors in Drug Design.	3
389	New Betulin Derivatives with Nitrogen Heterocyclic MoietySynthesis and Anticancer Activity In Vitro. **2022**, 12, 1540	0
388	Inhibition of PTP1B by isosinensetin, a polymethoxylated flavone isolated from trifoliate orange peel: kinetic studies, molecular docking, and molecular dynamics simulation.	0
387	Antileishmanial Activity of 4,8-Dimethoxynaphthalenyl Chalcones on Leishmania amazonensis. **2022**, 11, 1402	1
386	A Comprehensive Study to Unleash the Putative Inhibitors of Serotype2 of Dengue Virus: Insights from an In Silico Structure-Based Drug Discovery.	0

385	In silico investigations identified Butyl Xanalterate to competently target CK2 (CSNK2A1) for therapy of chronic lymphocytic leukemia. **2022**, 12,	3
384	ADME and DMPK considerations for the Discovery and Development of Antibody Drug Conjugates (ADCs). 1-44	0
383	Reactivity and binding mode of disulfiram, its metabolites, and derivatives in SARS-CoV-2 PLpro: insights from computational chemistry studies. **2022**, 28,	0
382	Fluorinated derivatives of tetrahydroaltersolanol molecule on COVID-19, HIV, and HTLV protease by DFT and molecular docking approaches. **2022**, 28,	0
381	Theoretical Studies, Spectroscopic Investigation, Molecular Docking, Molecular Dynamics and MMGBSA Calculations with 2-Hydrazinoquinoline. **2022**, 134482	0
380	In vitro effects of 2-methyl-3-propylbutane-1,4-diol purified from Alstonia boonei on erythrocyte membrane stabilisation and mitochondrial membrane permeabilisation.	1
379	Chemical profile of the pits oil from the Tunisian Aligu cultivar of Phoenix dactylifera L.: In vivo wound healing potential evaluation of a cream formulated from the extracted oil and insights from molecular docking and SAR analysis.	0
378	Screening the possible anti-cancer constituents of Hibiscus rosa-sinensis flower to address mammalian target of rapamycin: an in silico molecular docking, HYDE scoring, dynamic studies, and pharmacokinetic prediction.	0
377	LY3041658/ interleukin-8 complex structure as targets for IL-8 small molecule inhibitors discovery using a combination of in silico methods. 1-26	1
376	Emerging and advanced drug delivery systems for improved biopharmaceutical attributes of gallic acid: A review. **2022**, 2, 100369	0
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374	In silico study of local anesthetics analogues on sodium channel Nav 1.7 a pharmacological target on inflamed dental pulp. **2022**, 101117	0
373	ZnO Nanoparticle-Assisted Synthesis of Thiazolo[3,2- Pyrimidine Analogs: Antibacterial and Antioxidant Activity, In Silico Molecular Docking, and ADMET Prediction Study. **2022**, 2022, 1-20	0
372	Recent Advances of DprE1 Inhibitors against Mycobacterium tuberculosis: Computational Analysis of Physicochemical and ADMET Properties.	1
371	Flavonoids from Ericameria nauseosa inhibiting PI3K/AKT pathway in human melanoma cells. **2022**, 156, 113754	0
370	Recent trends in fragment-based anticancer drug design strategies against different targets: A mini-review. **2022**, 206, 115301	0
369	Network pharmacology-based elucidation of bioactive compounds in propolis and putative underlying mechanisms against type-2 diabetes mellitus. **2022**, 5, 100183	0
368	Seven-membered ring fused pyrimidine-based derivatives and their biological properties. **2023**, 249-263	0

367	Therapeutic potential of fucosyltransferases in cancer and recent development of targeted inhibitors. **2023**, 28, 103394	0
366	Nature-inspired new isoindole-based Passerini adducts as efficient tumor-selective apoptotic inducers via caspase-3/7 activation. **2023**, 245, 114865	0
365	In vitro cytotoxic effects, in silico studies, some metabolic enzymes inhibition, and vibrational spectral analysis of novel □amino alcohol compounds. **2023**, 1273, 134282	0
364	In silico pharmacokinetics, molecular docking and dynamic simulation studies of endolichenic fungi secondary metabolites: An implication in identifying novel kinase inhibitors as potential anticancer agents. **2023**, 1273, 134390	0
363	LEKI WIELOCELOWE □NOWY PARADYGMAT W PROJEKTOWANIU LEK□W. **2013**, 11, 1-10	0
362	Chapter 13. Ayurvedic Knowledge Inspired Approach to Modern Drug Discovery. **2022**, 325-373	0
361	Using filters in virtual screening: A comprehensive guide to minimize errors and maximize efficiency. **2022**,	0
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161	Facile synthesis and in-vitro cytotoxicity study of some 5-(4-substituted phenyl)-7-hydroxy-9-methyl-2-thioxo-2,3-dihydro-1H-dipyrimido[1,2-a:4?,5?-d]pyrimidin-4(5H)-one derivative and their Optoelectronic, DFT, and LFPs applications. **2023**, 1280, 135043	0
160	Exploration of Some Bis-Sulfide and Bis-Sulfone Derivatives as Non-Classical Aldose Reductase □hibitors. **2023**, 8,	0
159	Drug discovery: Standing on the shoulders of giants. **2023**, 207-338	0
158	2-[(2-Amino-6-methylpyrimidin-4-yl)sulfanyl]-N-arylacetamides: Discovery of a new class of anti-tubercular agents and prospects for their further structural modification. **2023**, 83, 129189	0
157	Identification of a PD1/PD-L1 inhibitor by Structure-Based Pharmacophore Modelling, Virtual Screening, Molecular docking and Biological Evaluation.	0
156	Antimicrobial potential of Chlorella sorokiniana on MRSA - an in vitro study and an in silico analysis on ClpP protease. **2023**, 102668	0
155	Synthesis, DFT calculations, and anti-proliferative evaluation of pyrimidine and selenadiazolopyrimidine derivatives as dual Topoisomerase II and HSP90 inhibitors. **2023**, 38,	0
154	Molecular Mechanism of the Therapeutic Effect of Peach Blossom against Constipation: An Exploratory Study Based on Network Pharmacology Analysis and Molecular Docking Verification. **2023**, 2023, 1-14	0
153	Novel Benzothiazole Derivatives Synthesis and its Analysis as Diuretic Agents. **2023**, 2023, 1-12	0
152	The promising guide to LC□MS analysis and cholinesterase activity of Luffa cylindrica (L.) fruit using in vitro and in-silico analyses. **2023**, 9,	0

151	Solid microemulsion preconcentrates on pH responsive metal-organic framework for tableting. **2023**, 186, 105-111	0
150	Computational probing of Nigella sativa bioactive metabolites against chickungunya nsP2 cysteine protease. **2023**, 35, 102651	0
149	N-aryl-2-(trifluoromethyl)benzo[b][1,8]naphthyridin-4(1H)-one as convenient platform to design high photostable and long-lived dyad fluorophore with potential application in live-cell imaging. **2023**, 439, 114619	0
148	Anti-inflammatory or anti-SARS-CoV-2 ingredients in Huashi Baidu Decoction and their corresponding targets: Target screening and molecular docking study. **2023**, 16, 104663	0
147	Synthesis of benzylidene-indandione derivatives as quantification of amyloid fibrils. **2023**, 296, 106982	0
146	Synthesis, characterization, antioxidant and antiparasitic activities new naphthyl-thiazole derivatives. **2023**, 248, 108498	0
145	Phytochemistry of the Vepris genus plants: A review and in silico analysis of their ADMET properties. **2023**, 157, 106-114	0
144	4-(4-methoxyphenyl)-6-methyl-3-phenyl-4H-1,2,4-oxadiazin-5(6H)-one: Synthesis, crystal structure, Hirshfeld surface analysis, noncovalent, ADMET studies and biological evaluation. **2023**, 1282, 135197	0
143	In silico prediction of Antifungal compounds from Natural sources towards Lanosterol 14-alpha demethylase (CYP51) using Molecular docking and Molecular dynamic simulation. **2023**, 121, 108435	0
142	Application of computational methods for class A GPCR Ligand discovery. **2023**, 121, 108434	0
141	Artificial intelligence in cancer immunotherapy: Applications in neoantigen recognition, antibody design and immunotherapy response prediction. **2023**, 91, 50-69	0
140	QSAR-based virtual screening of traditional Chinese medicine for the identification of mitotic kinesin Eg5 inhibitors. **2023**, 104, 107865	0
139	Docking Studies of Natural Product Derived Carvacrol Type Aromatic Monoterpenes Against COVID-19 and Comparison with Used Synthetic Drugs: Potential of Carvacryl Acetate Against SARS-CoV-2 (COVID-19). **2023**, 12, 1-14	0
138	Deep multi-agent fusion Q-Network for graph generation. **2023**, 269, 110509	0
137	New oxadiazole/triazole derivatives with antimicrobial and antioxidant properties. **2023**, 1282, 135213	1
136	Discovery of novel benzenesulfonamides incorporating 1,2,3-triazole scaffold as carbonic anhydrase I, II, IX, and XII inhibitors. **2023**, 239, 124232	0
135	Virtual screening, pharmacokinetic, and DFT studies of anticancer compounds as potential kinase inhibitors. **2023**, 18, 933-946	0
134	New flavone-based arylamides as potential V600E-BRAF inhibitors: Molecular docking, DFT, and pharmacokinetic properties. **2023**, 18, 1000-1010	0

133	Identification of some novel amide conjugates as potent and gastric sparing anti-inflammatory agents: In vitro, in vivo, in silico studies and drug safety evaluation. **2023**, 1285, 135521	0
132	Synthesis, in silico studies and investigations on antimicrobial, antimalarial activities of p-toluenesulphonamoyl Leu-Gly dipeptide carboxamide derivatives. **2023**, 1285, 135529	0
131	Effective bioactive compounds and their antiviral properties from some selected aquatic plants through in silico and in vitro approaches. **2023**, 573, 739574	0
130	Identifying non-nucleoside inhibitors of RNA-dependent RNA-polymerase of SARS-CoV-2 through per-residue energy decomposition-based pharmacophore modeling, molecular docking, and molecular dynamics simulation. **2023**, 16, 501-519	0
129	Tacrolimus and paclitaxel co-loaded O/O ointment without surfactant: Synergistic combinations for the treatment of psoriasis. **2023**, 185, 28-43	0
128	Current and emerging approaches to noncompetitive AR inhibition.	0
127	Insecticide discovery chance favors the prepared mind **2023**, 192, 105412	0
126	Structure-based identification of potential substrate antagonists for isethionate sulfite-lyase enzyme of Bilophila Wadsworthia: Towards novel therapeutic intervention to curb gut-associated illness. **2023**, 240, 124428	0
125	LigityScore: A CNN-Based Method for Binding Affinity Predictions. **2022**, 18-44	0
124	Discovery, synthesis and mechanism study of 2,3,5-substituted [1,2,4]-thiadiazoles as covalent inhibitors targeting 3C-Like protease of SARS-CoV-2. **2023**, 249, 115129	0
123	Physicochemical parameters for design and development of lead herbicide molecules: Is Lipinski's rule of 5? appropriate for herbicide discovery?. **2023**, 79, 1931-1943	0
122	Molecular docking with SARS-CoV-2 and potential drug property of a bioactive novel Zn(II) polymer: A combined experimental and theoretical study. **2023**, 233, 116304	0
121	Hit to lead optimization and chemoinformatic studies for a new series of Autotaxin inhibitors. **2023**, 249, 115130	0
120	Efficient synthesis of chromeno[2,3-b]pyridine derivatives using Zn(OTf)2 as a catalyst: DFT computations, molecular docking and ADME studies. **2023**, 375, 121364	0
119	Rational design of novel compounds to serve as potential NDM-1 inhibitors using molecular docking, molecular dynamics simulation, and physicochemical studies.	0
118	In Silico Drug Design and Analysis of Dual Amyloid-Beta and Tau Protein-Aggregation Inhibitors for Alzheimer's Disease Treatment. **2023**, 28, 1388	0
117	Synthesis, antifungal evaluation, and molecular docking studies of steroidal thiazolopyrimidines. **2023**, 193, 109186	0
116	Drug-Like Small Molecules That Inhibit Expression of the Oncogenic MicroRNA-21. **2023**, 18, 237-250	0

115	Complexity of the Role of Various Site-Specific and Selective Sudlow Binding Site Drugs in the Energetics and Stability of the Acridinedione Dye–Bovine Serum Albumin Complex: A Molecular Docking Approach. **2023**, 8, 5634-5654	0
114	Challenges Based on Antiplasmodial and Antiviral Activities of 7-Chloro-4-aminoquinoline Derivatives. **2023**, 18,	0
113	Identification of Promising Drug Candidates against Prostate Cancer through Computationally-Driven Drug Repurposing. **2023**, 24, 3135	0
112	Link-INVENT: generative linker design with reinforcement learning. **2023**, 2, 392-408	0
111	Instigating the in vitro antidiabetic activity of new tridentate Schiff base ligand appended M(II) complexes: From synthesis, structural characterization, quantum computational calculations to molecular docking, and molecular dynamics simulation studies. **2023**, 37,	0
110	Synthesis and Structure of 4-Aryl-3,6-dioxo-2,3,4,5,6,7-hexahydroisothiazolo[5,4-b]pyridine-5-carbonitriles. **2022**, 92, 2861-2869	1
109	Synthesis and Some Properties of 2-Amino-4-aryl-6-hexyl-7-hydroxy-4H-chromene-3-carbonitriles. **2022**, 92, 2850-2860	0
108	Identification of binding sites in nicastrin and binding modes of its inhibitors. 12, 150	0
107	Computational Evaluation of N-Based Transannular Interactions in Some Model Fused Medium-Sized Heterocyclic Systems and Implications for Drug Design. **2023**, 28, 1631	1
106	An integrated in-silico Pharmaco-BioInformatics approaches to identify synergistic effects of COVID-19 to HIV patients. **2023**, 155, 106656	0
105	Lessons for Oral Bioavailability: How Conformationally Flexible Cyclic Peptides Enter and Cross Lipid Membranes. **2023**, 66, 2773-2788	0
104	Potential Mechanisms of Yiqi Jiedu Huayu Decoction in the Treatment of Diabetic Microvascular Complications Based on Network Analysis, Molecular Docking, and Experimental Validation. **2023**, 2023, 1-19	0
103	ENZYMES IN HUMAN HEALTH. **2023**, 487-541	0
102	Bioactive compounds from four Indian medicinal plants have different potency to induce sex reversal in Nile tilapia: A chromatographic, molecular docking and in silico analysis. **2023**, 307, 116263	0
101	In silico studies, X-ray diffraction analysis and biological investigation of fluorinated pyrrolylated-chalcones in zebrafish epilepsy models. **2023**, 9, e13685	0
100	Structure-Aided Identification of an Inhibitor Targets Mps1 for the Management of Plant-Pathogenic Fungi.	1
99	Development of Combretastatin A-4 Analogues as Potential Anticancer Agents with Improved Aqueous Solubility. **2023**, 28, 1717	0
98	Solvent–solute interactions, electronic properties, topological and biological explorations of 6-Bromo-7-methylimidazo[1,2-a]pyridine. **2023**, 376, 121437	0

97	QSAR, ADME-Tox, molecular docking and molecular dynamics simulations of novel selective glycine transporter type 1 inhibitors with memory enhancing properties. **2023**, 9, e13706	0
96	In-silico study for African plants with possible beta-cell regeneration effect through inhibition of DYRK1A. **2022**, 1, 13-28	0
95	Unravelling the destabilization potential of ellagic acid on □synuclein fibrils using molecular dynamics simulations. **2023**, 25, 8128-8143	0
94	An Insight into Wheat Germ Oil Nutrition, Identification of Its Bioactive Constituents and Computer-Aided Multidimensional Data Analysis of Its Potential Anti-Inflammatory Effect via Molecular Connections. **2023**, 13, 526	2
93	Asymmetric Synthesis of Trisubstituted Piperidines via Biocatalytic Transamination and Diastereoselective Enamine or Imine Reduction.	0
92	Contamination of Sewage Water with Active Pharmaceutical Ingredients: An Emerging Threat to Food Products and Human Health. **2023**, 193-231	0
91	Development of a quaternary ammonium poly (amidoamine) dendrimer-based drug carrier for the solubility enhancement and sustained release of furosemide. 11,	0
90	In Vitro Antibacterial Efficacy of Cymbopogon flexuosus Essential Oil against Aeromonas hydrophila of Fish Origin and in Silico Molecular Docking of the Essential Oil Components against DNA Gyrase-B and Their Drug-Likeness. **2023**, 20,	0
89	Nigelladine A among Selected Compounds from Nigella sativa Exhibits Propitious Interaction with Omicron Variant of SARS-CoV-2: An In Silico Study. **2023**, 2023, 1-14	0
88	Delivering on the promise of protein degraders.	0
87	In vitro Assessment of Anti-Microbial Activity of Aloe vera (Barbadensis miller) Supported through Computational Studies.	0
86	Trust Your Gut: Strategies and Tactics for Intestinally Restricted Drugs. **2023**, 14, 233-243	0
85	Phenotypic Discovery of Thiocarbohydrazone with Anticancer Properties and Catalytic Inhibition of Human DNA Topoisomerase II□**2023**, 16, 341	0
84	Antiviral activity of Humulus lupulus (HOP) aqueous extract against MERS-CoV and SARS-CoV-2: in-vitro and in-silico study. **2023**, 37, 167-179	0
83	Eaton's reagent is an alternative of PPA: Solvent free synthesis, molecular docking and ADME studies of new angular and linear carbazole based naphtho naphthyridines. **2023**, 135, 133320	0
82	Molecular Docking approach on the effect of Site- Selective and Site-Specific Drugs on the Molecular Interactions of Human Serum Albumin (HSA) -Acridinedione dye complex. **2023**, 16, 104701	0
81	Triad pyrazole□hiazole□oumarin heterocyclic core effectively inhibit HSP and drive cancer cells to apoptosis. 1-16	0
80	Molecular Docking and ADMET Study of Spice-Derived Potential Phytochemicals against Human DNA Topoisomerase III Alpha. **2023**, 407,	0

79	Quantum Computational, Spectroscopic (FT-IR, FT-Raman, NMR, and UV–Vis) Hirshfeld Surface and Molecular Docking-Dynamics Studies on 5-Hydroxymethyluracil (Monomer and Trimer). **2023**, 28, 2116	0
78	Discovery of Antitrypanosomal Indolylacetamides by a Deconstruction–Optimization Strategy Applied to Paullones.	0
77	Synthesis and Biological Evaluation of Novel Uracil Derivatives as Thymidylate Synthase Inhibitors.	0
76	Indenyl-thiazole and indenyl-formazan derivatives: Synthesis, anticancer screening studies, molecular-docking, and pharmacokinetic/ molin-spiration properties. **2023**, 18, e0274459	1
75	Focusing on the moderately active compound (MAC) in the design and development of strategies to optimize the apoptotic effect by molecular mechanics techniques. **2023**, 1, 118-126	0
74	Exploring the Interaction Between the Newly Designed Antitumor Zn(II) Complex and CT-DNA/BSA: Spectroscopic Methods, DFT Computational Analysis, and Docking Simulation.	0
73	Synthesis of benzylidene-benzofuranone derivatives as probes for detection of amyloid fibrils in cells. 1-14	0
72	Synthesis of thiazolo[3,2-a]pyrimidine molecules, in vitro cytotoxic evaluation and molecular docking studies.	0
71	Structure-based discovery of cannabinoid-1 receptor agonists with reduced side effects.	0
70	Rapid and Efficient Access to Novel Bio-Inspired 3-Dimensional Tricyclic SpiroLactams as Privileged Structures via Meyers–Lactamization. **2023**, 16, 413	0
69	Antimicrobial Evaluation of New Pyrazoles, Indazoles and Pyrazolines Prepared in Continuous Flow Mode. **2023**, 24, 5319	0
68	Repurposing 1,2,4-oxadiazoles as SARS-CoV-2 PLpro inhibitors and investigation of their possible viral entry blockade potential. **2023**, 252, 115272	0
67	Fast calculation of hydrogen-bond strengths and free energy of hydration of small molecules. **2023**, 13,	0
66	Metabolic, toxicological, chemical, and commercial perspectives on esterification of dietary polyphenols: a review. 1-40	0
65	In-silico investigation and drug likeliness studies of benzimidazole congeners: The new face of innovation. **2023**, 38, 101213	0
64	Pharmaceutical Methods for Enhancing the Dissolution of Poorly Water-Soluble Drugs. **2023**, 21, 65-79	0
63	Dithiocarbamate-based linear versus macrocyclic architecture: comparative studies and applications in protein interaction and heavy metal removal.	0
62	Using Machine Learning To Predict Partition Coefficient (Log P) and Distribution Coefficient (Log D) with Molecular Descriptors and Liquid Chromatography Retention Time. **2023**, 63, 1906-1913	0

61	Structure-based small inhibitors search combined with molecular dynamics driven energies for human programmed cell death-1 (PD-1) protein. 1-15	1
60	Relevance of the Trillion-Sized Chemical Space □Xplore□ as a Source for Drug Discovery. **2023**, 14, 466-472	0
59	Preparation and Evaluation of 6-Gingerol Derivatives as Novel Antioxidants and Antiplatelet Agents. **2023**, 12, 744	0
58	Computational evaluation of bioactive compounds from Viscum album (mistletoe) as inhibitors of p63 for pancreatic cancer treatment. 1-15	0
57	Efficient screening of protein-ligand complexes in lipid bilayers using LoCoMock score. **2023**, 37, 217-225	0
56	Investigations of p-tolyloxy-1,3,4-oxadiazole propionamides as soybean 15-lipoxygenase inhibitors in comforting with in vitro and in silico studies. 1-20	0
55	Synthesis and Evaluation of some Novel Triazolo-thiadizoles Derivatives as Anti-diabetic Activity. **2023**, 1-7	0
54	Study of two combined series of triketones with HPPD inhibitory activity by molecular modelling. 1-16	0
53	Computational study of physicochemical, optical, and thermodynamic properties of 2,2-dimethylchromene derivatives. **2023**, 29,	0
52	Ibuprofen and Paracetamol when They Meet: Quantum Theory of Atoms in Molecules Perspective. **2023**, 44, 188-196	0
51	Gex2SGen: Designing Drug-like Molecules from Desired Gene Expression Signatures. **2023**, 63, 1882-1893	0
50	Hydrogen bonds of OC ? NH motif in rings in drugs: A molecular electrostatic potential analysis.	0
49	Food Toxicity of Mycotoxin Citrinin and Molecular Mechanisms of Its Potential Toxicity Effects through the Implicated Targets Predicted by Computer-Aided Multidimensional Data Analysis. **2023**, 13, 880	0
48	In silico modeling revealed phytomolecules derived from Cymbopogon citratus (DC.) leaf extract as promising candidates for malaria therapy. 1-18	0
47	Antioxidant enzyme activities, molecular docking studies, MM-GBSA, and molecular dynamic of chlorpyrifos in freshwater fish Capoeta umbla. 1-14	0
46	Small Molecule Degraders of Protein Tyrosine Phosphatase 1B and T-Cell Protein Tyrosine Phosphatase for Cancer Immunotherapy.	0
45	Small Molecule Degraders of Protein Tyrosine Phosphatase 1B and T-Cell Protein Tyrosine Phosphatase for Cancer Immunotherapy.	0
44	Binding mechanism of andrographolide with intramolecular antiparallel G-quadruplexes of therapeutic importance: an in-silico analysis. **2023**, 49, 816-828	0

43	Targeting Shikimate Kinase Pathway of Acinetobacter baumannii: A Structure-Based Computational Approach to Identify Antibacterial Compounds. **2023**, 2023, 1-14	0
42	Open Macromolecular Genome: Generative Design of Synthetically Accessible Polymers.	0
41	Absolute oral bioavailability and possible metabolic pathway of panduratin A from Boesenbergia rotunda extract in beagle dogs. **2023**, 61, 590-597	0
40	In Silico Analyses of a Promising Drug Candidate for the Treatment of Amyotrophic Lateral Sclerosis Targeting Superoxide Dismutase I Protein. **2023**, 15, 1095	0
39	In Silico Analysis of Bioactive Compounds from Sea Urchin (Echinometra mathaei) against SARS-COV-2. **2023**, 16, 329-337	0
38	Pharmacophoric Evaluation of Compounds Isolated from GC-MS Analytical Method of Aqueous Extract of Azadirachta indica Leaves. **2023**, 16, 451-465	0
37	Synthesis, Antiproliferative Effect and In Silico LogP Prediction of BIM-23052 Analogs Containing Tyr Instead of Phe. **2023**, 15, 1123	0
36	Novel asymmetrical azines appending 1,3,4-thiadiazole sulfonamide: synthesis, molecular structure analyses, in silico ADME, and cytotoxic effect. **2023**, 13, 10353-10366	0
35	Design, Synthesis, In-silico Studies and Antiproliferative Evaluation of Novel Indazole Derivatives as Small Molecule Inhibitors of B-Raf. **2023**, 8,	0
34	Anticancer activity, DFT study, ADMET prediction, and molecular docking of novel □sulfamidophosphonates.	0
33	Novel Benzo Five-Membered Heterocycle Derivatives as P-Glycoprotein Inhibitors: Design, Synthesis, Molecular Docking, and Anti-Multidrug Resistance Activity.	0
32	Magic Chloro□Profound Effects of the Chlorine Atom in Drug Discovery.	0
31	Macrocycles in Drug Discovery-Learning from the Past for the Future.	0
30	Proanthocyanidins in Pruning Wood Extracts of Four European Plum (Prunus domestica L.) Cultivars and Their h LDHA Inhibitory Activity.	0
29	Potent FOXO3a Activators from Biologically Active Compound Library for Cancer Therapeutics: An ĩn ́silico Approach.	0
28	Computational nanoscience and technology. **2023**, 12, 100147	0
27	Discovery of nontriterpenoids from the rot roots of Panax notoginseng with cytotoxicity and their molecular docking study and experimental validation. **2023**, 13, 11037-11043	0
26	Studies on crystal growth, experimental, structural, DFT, optical, thermal and biological studies of 3-hydroxy-4-methoxybenzaldehyde single crystals. **2023**, 9, e15219	0

25	A computational investigation of galactopyranoside esters as antimicrobial agents through antiviral, molecular docking, molecular dynamics, pharmacokinetics, and bioactivity prediction. 1-16	0
24	Between the Devil and the Deep Blue Sea: Resveratrol, Sulfotransferases and Sulfatases: A Long and Turbulent Journey from Intestinal Absorption to Target Cells. **2023**, 28, 3297	0
23	Inhibitory Potential of the Ocimum sanctum Phytochemicals on Bruton's Tyrosine Kinase, a Well-Known Drug Target for Treatment of Chronic Lymphocytic Leukemia: An In Silico Investigation. **2023**, 28, 3287	0
22	Synthesis and biological evaluation of biaryl alkyl ethers as inhibitors of IDO1. **2023**, 88, 129280	0
21	Discovery of First-in-Class Small Molecule Inhibitors of Lymphocyte Activation Gene 3 (LAG-3).	0
20	Phytochemical profiling, in vitro antioxidants, and antidiabetic efficacy of ethyl acetate fraction of Lespedeza cuneata on streptozotocin-induced diabetic rats.	0
19	Design, synthesis, anticancer, and antibacterial evaluation of some quinazolinone-based derivatives as DHFR inhibitors.	0
18	Mannich bases derivatives of 2-Phenyl-5-Benzimidazole sulfonic acid; Synthesis, Characterization, Computational studies and Biological evaluation. 59,	0
17	A Bayesian Method for Concurrently Designing Molecules and Synthetic Reaction Networks.	0
16	Novel 1,3-diaryltriazene-substituted sulfaguanidine derivatives as selective carbonic anhydrase inhibitors: Synthesis, characterization, inhibition effects, and molecular docking studies.	0
15	Exploration of limonoids for their broad spectrum antiviral potential via DFT, molecular docking and molecular dynamics simulation approach. 1-6	0
14	Multitargeted Virtual Screening and Molecular Simulation of Natural Product-like Compounds against GSK3, NMDA-Receptor, and BACE-1 for the Management of Alzheimer's Disease. **2023**, 16, 622	0
13	Exploring halophilic environments as a source of new antibiotics. 1-30	0
12	Computational approaches for anticancer drug design. **2023**, 1-10	0
11	Design, synthesis, molecular docking study and molecular dynamics simulation of new coumarin-pyrimidine hybrid compounds having anticancer and antidiabetic activity.	0
10	Homology Modeling, Screening, and Identification of Potential FOXO6 Inhibitors Curtail Gastric Cancer Progression: an In Silico Drug Repurposing Approach.	0
9	Multi-ligand functionalized blood-to-tumor sequential targeting strategies in the field of glioblastoma nanomedicine.	0
8	VirtualFlow 2.0 - The Next Generation Drug Discovery Platform Enabling Adaptive Screens of 69 Billion Molecules.	0

7	Synthesis and in vitro study of pyrimidine-phthalimide hybrids as VEGFR2 inhibitors with antiproliferative activity. **2023**, 15, 661-677	0
6	Pharmacological Characteristics of the Hydroethanolic Extract of Acmella oleracea (L) R. K. Jansen Flowers: ADME/Tox In Silico and In Vivo Antihypertensive and Chronic Toxicity Evaluation. **2023**, 2023, 1-16	0
5	Design, synthesis, and docking of novel thiazolidine-2,4-dione multitarget scaffold as new approach for cancer treatment.	0
4	Synthesis, X-ray diffraction and theoretical studies to understand the molecular basis of druglikeness of isoxazole analogs. **2023**, 1287, 135734	0
3	Spectroscopic characterization, electronic transitions and pharmacodynamic analysis of 1-Phenyl-1,3-butanedione: An effective agent for antipsychotic activity. **2023**, 6, 100226	0
2	GC-MS screening of the phytochemical composition of Ziziphus honey: ADME properties and in vitro/in silico study of its antimicrobial activity. 1-13	0
1	Synthesis of New Compounds Bearing Methyl Sulfonyl Pharmacophore As Selective COX -2 Inhibitor.	0