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The influence of drug-like concepts on  
decision-making in medicinal chemistry

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518	Mineralocorticoid Receptor Antagonists. <b>2019</b> , 109, 151-188	3

517	Predicting the Risks of Drug-Induced Liver Injury in Humans Utilizing Computational Modeling. <b>2019</b> , 259-278	
516	An overview on the synthetic and medicinal perspectives of indenopyrazoles. <b>2019</b> , 178, 1-12	8
515	The Invention of Grazoprevir: An HCV NS3/4a Protease Inhibitor. <b>2019</b> , 355-387	1
514	Synthesis and molecular modeling of novel non-sulfonylureas as hypoglycemic agents and selective ALR2 inhibitors. <b>2019</b> , 27, 3383-3389	6
513	Fragment-based drug design of nature-inspired compounds. <b>2019</b> , 4,	2
512	Successful oral delivery of poorly water-soluble drugs both depends on the intraluminal behavior of drugs and of appropriate advanced drug delivery systems. <b>2019</b> , 137, 104967	118
511	The Accordion Pill: unique oral delivery to enhance pharmacokinetics and therapeutic benefit of challenging drugs. <b>2019</b> , 10, 433-442	6
510	Exploring the Chemical Space of Cytochrome P450 Inhibitors Using Integrated Physicochemical Parameters, Drug Efficiency Metrics and Decision Tree Models. <b>2019</b> , 7, 26	3
509	Revealing Drug Self-Associations into Nano-Entities. <b>2019</b> , 4, 8919-8925	3
508	3-Arylindanones and related compounds as antiproliferative agents against colorectal cancer. <b>2019</b> , 94, 1694-1705	
507	Imidazole and Methoxybenzylamine Growth Inhibitors Reduce Persistence in Tomato Plant Tissues. <b>2019</b> , 82, 997-1006	4
506	Eigen Value ANalySis (EVANS) - A Tool to Address Pharmacodynamic, Pharmacokinetic and Toxicity Issues. <b>2019</b> , 4, 118-136	0
505	Discovery of a Thiadiazole-Pyridazine-Based Allosteric Glutaminase 1 Inhibitor Series That Demonstrates Oral Bioavailability and Activity in Tumor Xenograft Models. <b>2019</b> , 62, 6540-6560	13
504	Copper-catalyzed synthesis of 2-aminopyridylbenzoxazoles domino reactions of intermolecular -arylation and intramolecular -arylation.. <b>2019</b> , 9, 13414-13417	1
503	Offline preparative 2-D polar-copolymerized reversed-phase chromatography $\zeta$ witterionic hydrophilic interaction chromatography for effective purification of polar compounds from Caulis Polygoni Multiflori. <b>2019</b> , 1118-1119, 70-77	11
502	CFH, a Functional Group-Dependent Hydrogen-Bond Donor: Is It a More or Less Lipophilic Bioisostere of OH, SH, and CH?. <b>2019</b> , 62, 5628-5637	86
501	Nitroketene -,acetals: synergistic building blocks for the synthesis of heterocycles.. <b>2019</b> , 9, 14477-14502	25
500	Cu and Au Complexes with Glycoconjugated Dithiocarbamate Ligands for Potential Applications in Targeted Chemotherapy. <b>2019</b> , 14, 1162-1172	11

499	High-throughput screening of the Plasmodium falciparum cGMP-dependent protein kinase identified a thiazole scaffold which kills erythrocytic and sexual stage parasites. <b>2019</b> , 9, 7005	25
498	An efficient microwave-promoted three-component synthesis of thiazolo[3,2-a]pyrimidines catalyzed by SiO <sub>2</sub> ZnBr <sub>2</sub> and antimicrobial activity evaluation. <b>2019</b> , 55, 266-274	3
497	Cheminformatics techniques in antimalarial drug discovery and development from natural products 1: basic concepts. <b>2019</b> , 4,	1
496	Proteolysis targeting chimeras (PROTACs) in 'beyond rule-of-five' chemical space: Recent progress and future challenges. <b>2019</b> , 29, 1555-1564	127
495	Discovery of 2-phenoxyacetamides as inhibitors of the Wnt-depalmitoleating enzyme NOTUM from an X-ray fragment screen. <b>2019</b> , 10, 1361-1369	17
494	UPLC-HRMS and NMR applied in the evaluation of solid-phase extraction methods as a rational strategy of dereplication of Phyllanthus spp. aiming at the discovery of cytotoxic metabolites. <b>2019</b> , 1120, 51-61	5
493	Benzoic acid-derived nitrones: A new class of potential acetylcholinesterase inhibitors and neuroprotective agents. <b>2019</b> , 174, 116-129	19
492	Discovery and Mechanistic Study of Tailor-Made Quinoline Derivatives as Topoisomerase 1 Poison with Potent Anticancer Activity. <b>2019</b> , 62, 3428-3446	37
491	Characterization of Drug-like Chemical Space for Cytotoxic Marine Metabolites Using Multivariate Methods. <b>2019</b> , 4, 5402-5411	8
490	Beyond the Flavour: The Potential Druggability of Chemosensory G Protein-Coupled Receptors. <b>2019</b> , 20,	37
489	DFT and QSAR investigations of substituent effects in pyrazolooxazine derivatives: Activity prediction. <b>2019</b> , 18, 1950001	2
488	In Silico Modeling of FDA-Approved Drugs for Discovery of Therapies Against Neglected Diseases: A Drug Repurposing Approach. <b>2019</b> , 625-648	3
487	EASL Clinical Practice Guidelines: Drug-induced liver injury. <b>2019</b> , 70, 1222-1261	327
486	Small molecules as central nervous system therapeutics: old challenges, new directions, and a philosophic divide. <b>2019</b> , 11, 489-493	16
485	Properties of FDA-approved small molecule protein kinase inhibitors. <b>2019</b> , 144, 19-50	247
484	Structures and anticancer activity of chlorido platinum(II) saccharinate complexes with mono- and dialkylphenylphosphines. <b>2019</b> , 195, 39-50	14
483	Seleno-Michael Reaction of Stable Functionalised Alkyl Selenols: A Versatile Tool for the Synthesis of Acyclic and Cyclic Unsymmetrical Alkyl and Vinyl Selenides. <b>2019</b> , 361, 2337-2346	26
482	A combinatorial approach for the discovery of drug-like inhibitors of 15-lipoxygenase-1. <b>2019</b> , 174, 45-55	8

481	Synthesis of novel amides, characterization by spectrometric methods, cytotoxic activity and theoretical calculations. <b>2019</b> , 1191, 6-16	1
480	QSAR Modeling and Drug-Likeness Screening for Antioxidant Activity of Benzofuran Derivatives. <b>2019</b> , 1189, 307-314	11
479	Novel Chemical Series of 5-Lipoxygenase-Activating Protein Inhibitors for Treatment of Coronary Artery Disease. <b>2019</b> , 62, 4325-4349	7
478	Metal-Free Photocatalysts for C-H Bond Oxygenation Reactions with Oxygen as the Oxidant. <b>2019</b> , 12, 2898-2910	58
477	Accelerated drug discovery by rapid candidate drug identification. <b>2019</b> , 24, 1237-1241	14
476	Biased Complement Diversity Selection for Effective Exploration of Chemical Space in Hit-Finding Campaigns. <b>2019</b> , 59, 1709-1714	4
475	Axially Chiral Cyclic Phosphoric Acid Enabled Enantioselective Sequential Additions. <b>2019</b> , 21, 2498-2503	14
474	Targeting ERK1/2 protein-serine/threonine kinases in human cancers. <b>2019</b> , 142, 151-168	100
473	Synthesis of quinazolin-4(1H)-ones via amination and annulation of amidines and benzamides. <b>2019</b> , 17, 2356-2360	6
472	Hypoxia-activated prodrugs and (lack of) clinical progress: The need for hypoxia-based biomarker patient selection in phase III clinical trials. <b>2019</b> , 15, 62-69	52
471	Structure-Based Design of N-(5-Phenylthiazol-2-yl)acrylamides as Novel and Potent Glutathione S-Transferase Omega 1 Inhibitors. <b>2019</b> , 62, 3068-3087	10
470	Discovery, synthesis and molecular corroborations of medicinally important novel pyrazoles; drug efficacy determinations through in silico, in vitro and cytotoxicity validations. <b>2019</b> , 86, 410-419	11
469	Mind and machine in drug design. <b>2019</b> , 1, 128-130	30
468	Drug-Induced Liver Disease: Mechanism and Diagnosis. <b>2019</b> , 715-728	1
467	Identification of Isoform-Selective Ligands for the Middle Domain of Heat Shock Protein 90 (Hsp90). <b>2019</b> , 20,	11
466	Proline-Based Allosteric Inhibitors of Zika and Dengue Virus NS2B/NS3 Proteases. <b>2019</b> , 62, 11359-11382	35
465	Carboranylanylinoquinazoline EGFR-inhibitors: toward 'lead-to-candidate' stage in the drug-development pipeline. <b>2019</b> , 11, 2273-2285	10
464	(3 + 1) Annulation/Rearrangement Cascade of $\alpha$ -Cyclic Azomethine Imines and 3-Chlorooxindoles: Construction of Hexahydroindeno[2,1- <i>b</i> ]pyrazole Spirooxindole Frameworks. <b>2019</b> , 21, 10052-10056	9

463	Revisiting the structure of a synthetic somatostatin analogue for peptide drug design. <b>2019</b> , 75, 611-620	7
462	Synergistic catalysis on Fe-N sites and Fe nanoparticles for efficient synthesis of quinolines and quinazolinones oxidative coupling of amines and aldehydes. <b>2019</b> , 10, 10283-10289	50
461	Pharmacological and SAR analysis of the LINS01 compounds at the human histamine H <sub>1</sub> , H <sub>2</sub> , and H <sub>3</sub> receptors. <b>2019</b> , 93, 89-95	4
460	Screening Strategies and Methods for Better Off-Target Liability Prediction and Identification of Small-Molecule Pharmaceuticals. <b>2019</b> , 24, 1-24	17
459	Synthesis approach and biological activity evaluation of a series of 1,3,2-oxazaphosphole-2-oxides against inflammation and nociception. <b>2019</b> , 150, 283-294	0
458	Novel, potent, selective, and brain penetrant phosphodiesterase 10A inhibitors. <b>2019</b> , 29, 406-412	2
457	Identification of novel uracil derivatives incorporating benzoic acid moieties as highly potent Dipeptidyl Peptidase-IV inhibitors. <b>2019</b> , 27, 644-654	10
456	Discovery of naldemedine: A potent and orally available opioid receptor antagonist for treatment of opioid-induced adverse effects. <b>2019</b> , 29, 73-77	8
455	Thiazole, thio and semicarbazone derivatives against tropical infective diseases: Chagas disease, human African trypanosomiasis (HAT), leishmaniasis, and malaria. <b>2019</b> , 162, 378-395	32
454	Optimization of a 1,3,4-oxadiazole series for inhibition of Ca/calmodulin-stimulated activity of adenylyl cyclases 1 and 8 for the treatment of chronic pain. <b>2019</b> , 162, 568-585	9
453	Analysis of solvent-exposed and buried co-crystallized ligands: a case study to support the design of novel protein-protein interaction inhibitors. <b>2019</b> , 24, 551-559	11
452	Fragment-to-Lead Medicinal Chemistry Publications in 2017. <b>2019</b> , 62, 3857-3872	27
451	Synthesis of New Potential Lipophilic Co-Drugs of 2-Chloro-2'-deoxyadenosine (Cladribine, 2-CdA, Mavencladine, Leustatin) and 6-Azauridine (z U) with Valproic Acid. <b>2019</b> , 16, e1800497	1
450	Visualize Embryogenesis and Cell Fate Using Fluorescent Probes with Aggregation-Induced Emission. <b>2019</b> , 11, 3737-3744	9
449	In vitro and in silico inhibition properties of fucoidan against $\alpha$ -amylase and $\beta$ -D-glucosidase with relevance to type 2 diabetes mellitus. <b>2019</b> , 209, 350-355	55
448	Computer-aided design, synthesis and biological characterization of novel inhibitors for PKMYT1. <b>2019</b> , 161, 479-492	11
447	Investigation of the molecular characteristics of bisindole inhibitors as HIV-1 glycoprotein-41 fusion inhibitors. <b>2019</b> , 161, 533-542	5
446	Structure-based exploration and pharmacological evaluation of N-substituted piperidin-4-yl-methanamine CXCR4 chemokine receptor antagonists. <b>2019</b> , 162, 631-649	8

445	Discovery of potent azaindazole leucine-rich repeat kinase 2 (LRRK2) inhibitors possessing a key intramolecular hydrogen bond - Part 2. <b>2019</b> , 29, 674-680	3
444	Population Balance Model for Simulation of the Supersaturation-Precipitation Behavior of Drugs in Supersaturable Solid Forms. <b>2019</b> , 108, 260-267	5
443	Discovery of potent and selective 5-azaindazole inhibitors of leucine-rich repeat kinase 2 (LRRK2) - Part 1. <b>2019</b> , 29, 668-673	3
442	Identification of Selective Acyl Sulfonamide-Cycloalkylether Inhibitors of the Voltage-Gated Sodium Channel (Na) 1.7 with Potent Analgesic Activity. <b>2019</b> , 62, 908-927	20
441	Discovery of Allosteric, Potent, Subtype Selective, and Peripherally Restricted TrkA Kinase Inhibitors. <b>2019</b> , 62, 247-265	27
440	Virtual screening in drug-likeness and structure/activity relationship of pyridazine derivatives as Anti-Alzheimer drugs. <b>2019</b> , 31, 595-601	17
439	Dynamic structure based pharmacophore modeling of the Acetylcholinesterase reveals several potential inhibitors. <b>2019</b> , 37, 1800-1812	26
438	Prediction of volume of distribution in humans: analysis of eight methods and their application in drug discovery. <b>2020</b> , 50, 270-279	8
437	Evaluation of the inhibitory effect of caffeic acid and gallic acid on tetR and tetM efflux pumps mediating tetracycline resistance in <i>Streptococcus</i> sp., using computational approach. <b>2020</b> , 32, 904-909	3
436	An Overview of Machine Learning and Big Data for Drug Toxicity Evaluation. <b>2020</b> , 33, 20-37	49
435	Alteration of Physicochemical Properties for Antibody-Drug Conjugates and Their Impact on Stability. <b>2020</b> , 109, 161-168	8
434	Small-Scale Panel Comprising Diverse Gene Family Targets To Evaluate Compound Promiscuity. <b>2020</b> , 33, 154-161	5
433	Modifying the lipophilic part of phenylthiazole antibiotics to control their drug-likeness. <b>2020</b> , 185, 111830	11
432	Promiscuity of in Vitro Secondary Pharmacology Assays and Implications for Lead Optimization Strategies. <b>2020</b> , 63, 6251-6275	7
431	Scaffold-hopping identifies furano[2,3-d]pyrimidine amides as potent Notum inhibitors. <b>2020</b> , 30, 126751	9
430	Application of Negative Design To Design a More Desirable Virtual Screening Library. <b>2020</b> , 63, 4411-4429	14
429	Influence of polymeric excipients on the solubility of aspirin: Experimental measurement and model prediction. <b>2020</b> , 508, 112450	5
428	Fragment-to-Lead Medicinal Chemistry Publications in 2018. <b>2020</b> , 63, 4430-4444	37

427	Gemini basic ionic liquid as bi-functional catalyst for the synthesis of 2,3-dihydroquinazolin-4(1H)-ones at room temperature. <b>2020</b> , 61, 151587	13
426	Properties of FDA-approved small molecule protein kinase inhibitors: A 2020 update. <b>2020</b> , 152, 104609	244
425	Is there enough focus on lipophilicity in drug discovery?. <b>2020</b> , 15, 261-263	19
424	Thermodynamic profiling for fragment-based lead discovery and optimization. <b>2020</b> , 15, 117-129	2
423	An in vitro toolbox to accelerate anti-malarial drug discovery and development. <b>2020</b> , 19, 1	72
422	Alkyne Linchpin Strategy for Drug:Pharmacophore Conjugation: Experimental and Computational Realization of a -Selective Inverse Sonogashira Coupling. <b>2020</b> , 142, 3762-3774	56
421	Docking Finds GPCR Ligands in Dark Chemical Matter. <b>2020</b> , 63, 613-620	11
420	Highly Dispersed Single-Phase Ni <sub>2</sub> P Nanoparticles on N,P-Codoped Porous Carbon for Efficient Synthesis of N-Heterocycles. <b>2020</b> , 8, 267-277	24
419	The blood-brain barrier: Physiology and strategies for drug delivery. <b>2020</b> , 165-166, 1-14	104
418	Design, synthesis, biological evaluation and molecular modeling of novel 1H-pyrrolo[2,3-b]pyridine derivatives as potential anti-tumor agents. <b>2020</b> , 94, 103474	10
417	Application of Hammett equation to hydrogen bond interactions of benzoic acid in chloroform/water system and explanation for non-linear Hammett relation to partition coefficients for the same system. <b>2020</b> , 1190, 113024	2
416	Chemoinformatic Approach: The Case of Natural Products of Panama. <b>2020</b> ,	2
415	. <b>2020</b> ,	0
414	3-Hetarylisocoumarins in the synthesis of 1-functionalized 3-hetarylisoquinolines. <b>2020</b> , 56, 1021-1029	1
413	preADMET analysis and clinical aspects of dogs treated with the Organotellurium compound RF07: A possible control for canine visceral leishmaniasis?. <b>2020</b> , 80, 103470	12
412	Fragment-based lead discovery of a novel class of small molecule antagonists of neuropeptide B/W receptor subtype 1 (GPR7). <b>2020</b> , 30, 127510	5
411	A Retrospective Biopharmaceutical Analysis of >800 Approved Oral Drug Products: Are Drug Properties of Solid Dispersions and Lipid-Based Formulations Distinctive?. <b>2020</b> , 109, 3248-3261	8
410	Cyanobacterial metabolites as promising drug leads against the M and PL of SARS-CoV-2: an analysis. <b>2021</b> , 39, 6218-6230	24



409	Synergistic potential of Citrus aurantium L. essential oil with antibiotics against Candida albicans. <b>2020</b> , 262, 113135	26
408	Novel phenethylimidazolium based ionic liquids: Design, microwave synthesis, in-silico, modeling and biological evaluation studies. <b>2020</b> , 315, 113778	10
407	Liver says no: the ongoing search for safe catechol O-methyltransferase inhibitors to replace tolcapone. <b>2020</b> , 25, 1846-1854	5
406	Pharmacokinetics (ADME). <b>2020</b> , 133-224	
405	Relevance of physicochemical properties and functional pharmacology data to predict the clinical safety profile of direct oral anticoagulants. <b>2020</b> , 8, e00603	7
404	Indole Propionic Acid, an Unusual Antibiotic Produced by the Gut Microbiota, With Anti-inflammatory and Antioxidant Properties. <b>2020</b> , 11, 575586	17
403	Fragment-to-Lead Medicinal Chemistry Publications in 2019. <b>2020</b> , 63, 15494-15507	18
402	EST64454: a Highly Soluble $\mu$ Receptor Antagonist Clinical Candidate for Pain Management. <b>2020</b> , 63, 14979-14988	3
401	Combinatorial Biosynthesis of Sulfated Benzenediol Lactones with a Phenolic Sulfotransferase from Fusarium graminearum PH-1. <b>2020</b> , 5,	4
400	Highly Potent and Selective $\gamma$ -Aryl Oxamic Acid-Based Inhibitors for Protein Tyrosine Phosphatase B. <b>2020</b> , 63, 9212-9227	9
399	A Phosphoramidate Strategy Enables Membrane Permeability of a Non-nucleotide Inhibitor of the Prolyl Isomerase Pin1. <b>2020</b> , 11, 1704-1710	2
398	Identification and Optimization of Pyrrolidine Derivatives as Highly Potent Ghrelin Receptor Full Agonists. <b>2020</b> , 63, 9705-9730	4
397	Harnessing emerging paradigms in chemical engineering to accelerate the development of pharmaceutical products. <b>2020</b> , 98, 2294-2300	0
396	Screening of a Custom-Designed Acid Fragment Library Identifies 1-Phenylpyrroles and 1-Phenylpyrrolidines as Inhibitors of Notum Carboxylesterase Activity. <b>2020</b> , 63, 9464-9483	7
395	Novel scaffold hopping of potent benzothiazole and isatin analogues linked to 1,2,3-triazole fragment that mimic quinazoline epidermal growth factor receptor inhibitors: Synthesis, antitumor and mechanistic analyses. <b>2020</b> , 103, 104133	20
394	Synthesis of Degraded Limonoid Analogs as New Antibacterial Scaffolds against. <b>2020</b> , 9,	0
393	Sulfoximines as Rising Stars in Modern Drug Discovery? Current Status and Perspective on an Emerging Functional Group in Medicinal Chemistry. <b>2020</b> , 63, 14243-14275	69
392	Potent and Selective Human Prostaglandin F (FP) Receptor Antagonist (BAY-6672) for the Treatment of Idiopathic Pulmonary Fibrosis (IPF). <b>2020</b> , 63, 11639-11662	4

391	Structure-based optimisation of orally active & reversible MetAP-2 inhibitors maintaining a tight 'molecular budget'. <b>2020</b> , 30, 127533	1
390	A [3 + 2] cycloaddition/C-arylation of isatin, $\alpha$ -cyclic azomethine imine 1,3-dipole with arynes.. <b>2020</b> , 10, 30620-30623	6
389	Diversity-Oriented Synthesis of Thiazolidine-2-imines via Microwave-Assisted One-Pot, Telescopic Approach and Its Interaction with Biomacromolecules. <b>2020</b> , 22, 630-640	5
388	Evaluation of DNA Binding and Topoisomerase I Inhibitory Activities of 16 $\beta$ -Decarbomethoxydihydrovoacamine from <i>Tabernaemontana corymbosa</i> . <b>2020</b> , 5, 14839-14843	1
387	Mono-Alkylated Ligands Based on Pyrazole and Triazole Derivatives Tested Against . sp. : Synthesis, Characterization, DFT, and Phytase Binding Site Identification Using Blind Docking/Virtual Screening for Potent Fophy Inhibitors. <b>2020</b> , 8, 559262	4
386	Inhibitors of dipeptidyl peptidase-4 as therapeutic agents for individuals with type 2 diabetes: a 25-year journey. <b>2020</b> , 37, 1230-1233	5
385	(E)-2-(2-Allylidenehydrazinyl)thiazole derivatives: Design, green synthesis, in silico and in vitro antimycobacterial and radical scavenging studies. <b>2020</b> , 353, e2000003	7
384	Design, synthesis and antiproliferative activity of new amine, amino acid and dipeptide-coupled benzamides as potential sigma-1 receptor. <b>2020</b> , 17, 2515-2532	10
383	Druggability and drug-likeness concepts in drug design: are biomodelling and predictive tools having their say?. <b>2020</b> , 26, 120	18
382	Design and Synthesis of Styrenylcyclopropylamine LSD1 Inhibitors. <b>2020</b> , 11, 1213-1220	10
381	Theoretical studies and NMR assay of coumarins and neoflavanones derivatives as potential inhibitors of acetylcholinesterase. <b>2020</b> , 87, 107293	1
380	Structure guided design of potent indole-based ATX inhibitors bearing hydrazone moiety with tumor suppression effects. <b>2020</b> , 201, 112456	3
379	Base-promoted Lewis acid catalyzed synthesis of quinazoline derivatives. <b>2020</b> ,	5
378	Serendipitous Synthesis of Pyridoquinazolinones an Oxidative C-C Bond Cleavage. <b>2020</b> , 85, 8102-8110	10
377	Synthesis, characterization and catalytic application of tributyl(carboxymethyl)phosphonium bromotrichloroferrate as a new magnetic ionic liquid for the preparation of 2,3-dihydroquinazolin-4(1H)-ones and 4H-pyrimidobenzothiazoles. <b>2020</b> , 46, 3945-3960	4
376	Synthesis and Structure-Activity Relationships of 5'-Aryl-14-alkoxypridomorphinans: Identification of a $\mu$ Opioid Receptor Agonist/ $\mu$ Opioid Receptor Antagonist Ligand with Systemic Antinociceptive Activity and Diminished Opioid Side Effects. <b>2020</b> , 63, 7663-7694	7
375	Stabilizing Inactive Conformations of MALT1 as an Effective Approach to Inhibit Its Protease Activity. <b>2020</b> , 3, 2000078	2
374	Didactic approach recounting advances and limitations in novel glutathione and cysteine detection (reduced GSH probe) with mixed coumarin, aldehyde, and phenyl-selenium chemistry. <b>2020</b> , 640, 267-289	4

373	Discovery of New Apoptosis-Inducing Agents for Breast Cancer Based on Ethyl 2-Amino-4,5,6,7-Tetra Hydrobenzo[ <i>b</i> ]Thiophene-3-Carboxylate: Synthesis, In Vitro, and In Vivo Activity Evaluation. <b>2020</b> , 25,	25
372	Combining Cloud-Based Free-Energy Calculations, Synthetically Aware Enumerations, and Goal-Directed Generative Machine Learning for Rapid Large-Scale Chemical Exploration and Optimization. <b>2020</b> , 60, 4311-4325	15
371	Structure-Based Design and Preclinical Characterization of Selective and Orally Bioavailable Factor XIa Inhibitors: Demonstrating the Power of an Integrated S1 Protease Family Approach. <b>2020</b> , 63, 8088-8113	7
370	Discovery of a Janus Kinase Inhibitor Bearing a Highly Three-Dimensional Spiro Scaffold: JTE-052 (Delgocitinib) as a New Dermatological Agent to Treat Inflammatory Skin Disorders. <b>2020</b> , 63, 7163-7185	17
369	Design, Synthesis, and Physicochemical and Pharmacological Profiling of 7-Hydroxy-5-oxopyrazolo[4,3- <i>b</i> ]pyridine-6-carboxamide Derivatives with Antiosteoarthritic Activity In Vivo. <b>2020</b> , 63, 7369-7391	11
368	Systems Pharmacology-Dissection of the Molecular Mechanisms of Dragon's Blood in Improving Ischemic Stroke Prognosis. <b>2020</b> , 2020, 4858201	1
367	Computational methods and tools for sustainable and green approaches in drug discovery. <b>2020</b> , 965-988	1
366	Synthetic approaches toward small molecule libraries. <b>2020</b> , 1-34	1
365	Synthetic and antimicrobial studies of N-substituted-pyrazoline-based new bisheterocycles. <b>2020</b> , 57, 2024-2036	2
364	Benzimidazoquinazolines as new potent anti-TB chemotypes: Design, synthesis, and biological evaluation. <b>2020</b> , 99, 103774	17
363	Molecular Iodine-Promoted [3 + 2] Oxidative Cyclization for the Synthesis of Heteroarene-Fused [1,2,4] Thiadiazoles/Selenadiazoles. <b>2020</b> , 85, 5570-5579	5
362	Identification of novel and selective agonists for ABA receptor PYL3. <b>2020</b> , 154, 387-395	10
361	Discovery of 2,4-diaminopyrimidine derivatives targeting p21-activated kinase 4: Biological evaluation and docking studies. <b>2020</b> , 353, e2000097	5
360	p-TSA.HO mediated one-pot, multi-component synthesis of isatin derived imidazoles as dual-purpose drugs against inflammation and cancer. <b>2020</b> , 102, 104046	9
359	Structure-guided optimization of a novel class of ASK1 inhibitors with increased sp character and an exquisite selectivity profile. <b>2020</b> , 30, 127405	4
358	Design of iodinated radioligands for SPECT imaging of central human 5-HTR using a ligand lipophilicity efficiency approach. <b>2020</b> , 96, 103582	1
357	Striking essential oil: tapping into a largely unexplored source for drug discovery. <b>2020</b> , 10, 2867	11
356	Cutaneous Adverse Events Caused by Sulfonamide-Containing Drugs: Reality or Perception?. <b>2020</b> , 63, 7447-7457	7

355	A Novel Systematic Approach for Selection of Prodrugs Designed to Improve Oral Absorption. <b>2020</b> , 109, 1736-1746	2
354	Electronic complementarity permits hindered butenolide heterodimerization and discovery of novel cGAS/STING pathway antagonists. <b>2020</b> , 12, 310-317	16
353	Development of a Novel Cell-Permeable Protein-Protein Interaction Inhibitor for the Polo-box Domain of Polo-like Kinase 1. <b>2020</b> , 5, 822-831	3
352	Lipophilic Metabolic Efficiency (LipMetE) and Drug Efficiency Indices to Explore the Metabolic Properties of the Substrates of Selected Cytochrome P450 Isoforms. <b>2020</b> , 5, 179-188	4
351	Cystobactamid 507: Concise Synthesis, Mode of Action, and Optimization toward More Potent Antibiotics. <b>2020</b> , 26, 7219-7225	10
350	Combining Structural, Thermodynamic, and Kinetic Information to Drive Hit-to-Lead Progression. <b>2020</b> , 99-124	1
349	Prediction of octanol-water partition coefficients for the SAMPL6-[Formula: see text] molecules using molecular dynamics simulations with OPLS-AA, AMBER and CHARMM force fields. <b>2020</b> , 34, 543-560	18
348	Vascular Epiphytic Medicinal Plants as Sources of Therapeutic Agents: Their Ethnopharmacological Uses, Chemical Composition, and Biological Activities. <b>2020</b> , 10,	18
347	Utility of Physicochemical Properties for the Prediction of Toxicological Outcomes: Takeda Perspective. <b>2020</b> , 11, 203-209	8
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344	The discovery, design and synthesis of potent agonists of adenylyl cyclase type 2 by virtual screening combining biological evaluation. <b>2020</b> , 191, 112115	4
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342	A Review on Recent Advances in Nitrogen-Containing Molecules and Their Biological Applications. <b>2020</b> , 25,	262
341	Treating Cancer by Spindle Assembly Checkpoint Abrogation: Discovery of Two Clinical Candidates, BAY 1161909 and BAY 1217389, Targeting MPS1 Kinase. <b>2020</b> , 63, 8025-8042	10
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338	Data science-driven analyses of drugs inducing hypertension as an adverse effect. <b>2021</b> , 25, 801-810	1

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336	Novel potent (dihydro)benzofuranyl piperazines as human histamine receptor ligands - Functional characterization and modeling studies on H and H receptors. <b>2021</b> , 30, 115924	3
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326	Put a ring on it: application of small aliphatic rings in medicinal chemistry. <b>2021</b> , 12, 448-471	43
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324	Novel Tandem Three Consecutive Reactions: Aza-Wittig, Imine Condensation and Electrophilic Aromatic Substitution Strategy to Indolizine Synthesis. <b>2021</b> , 11, 55-71	
323	Imidazopyridine-Based 5-HT Receptor Neutral Antagonists: Impact of -Benzyl and -Phenylsulfonyl Fragments on Different Receptor Conformational States. <b>2021</b> , 64, 1180-1196	9
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313	Metabolite profile of <i>Nectandra oppositifolia</i> Nees & Mart. and assessment of antitrypanosomal activity of bioactive compounds through efficiency analyses. <b>2021</b> , 16, e0247334	1
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304	Recent Experimental Developments in Studying Passive Membrane Transport of Drug Molecules. <b>2021</b> , 18, 2122-2141	5
303	Structure-Based Drug Design for G Protein-Coupled Receptors. 1-59	
302	Discovery of novel Hsp90 C-terminal domain inhibitors that disrupt co-chaperone binding. <b>2021</b> , 38, 127857	3

301	New Succinimides with Potent Anticancer Activity: Synthesis, Activation of Stress Signaling Pathways and Characterization of Apoptosis in Leukemia and Cervical Cancer Cells. <b>2021</b> , 22,	1
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296	Recent Advances in Chemistry Technologies and Applications to Medicinal Chemistry. 1-78	
295	Focused Libraries for Epigenetic Drug Discovery: The Importance of Isosteres. <b>2021</b> , 64, 7231-7240	6
294	Identification of Potent, Selective, and Orally Bioavailable Small-Molecule GSPT1/2 Degradors from a Focused Library of Cereblon Modulators. <b>2021</b> , 64, 7296-7311	10
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267	Amino-Substituted 3-Aryl- and 3-Heteroarylquinolines as Potential Antileishmanial Agents. <b>2021</b> , 64, 12152-12162	0
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257	Structure-Based Design and Discovery of Pyridyl-Bearing Fused Bicyclic HIV-1 Inhibitors: Synthesis, Biological Characterization, and Molecular Modeling Studies. <b>2021, 64, 13604-13621</b>	1
256	Discovery of 5-{4-[(7-Ethyl-6-oxo-5,6-dihydro-1,5-naphthyridin-3-yl)methyl]piperazin-1-yl}-methylpyridine-2-carboxamide (AZD5305): A PARP1-DNA Trapper with High Selectivity for PARP1 over PARP2 and Other PARPs. <b>2021, 64, 14498-14512</b>	8
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232	Attrition in Drug Discovery and Development. 5-45	2
231	What Does an HTS File of the Future Look Like?. 275-304	2
230	Generating a High-Quality Compound Collection. 9-21	3

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183	Medicinal Chemistry Strategies to Prevent Compound Attrition. 215-228	
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164	Combined Pharmacophore and Grid-Independent Molecular Descriptors (GRIND) Analysis to Probe 3D Features of Inositol 1,4,5-Trisphosphate Receptor (IPR) Inhibitors in Cancer. <b>2021</b> , 22,	2
163	Discovery of N-(2-benzyl-4-oxochroman-7-yl)-2-(5-(ethylsulfonyl) pyridin-2-yl) acetamide (b12) as a potent, selective, and orally available novel retinoic acid receptor-related orphan receptor $\beta$ inverse agonist.. <b>2021</b> , 119, 105483	1
162	Gold(I) Complexes with P-Donor Ligands and Their Biological Evaluation. <b>2021</b> , 9, 2100	
161	Molecular target prediction and docking of anti-thrombosis compounds and its activation on tissue-plasminogen activator to treat stroke. <b>2021</b> , 34, 101732	1
160	Computational Study on Potential Novel Anti-Ebola Virus Protein VP35 Natural Compounds.. <b>2021</b> , 9,	3
159	Recent Trends for Drug Development for the treatment of Adenocarcinoma breast cancer: Thiazole, Triazole, and Thiosemicarbazone Analogues as Efficient Scaffolds. <b>2021</b> ,	0
158	Discovery of 2H-chromone-4-one based sulfonamide derivatives as potent retinoic acid receptor-related orphan receptor $\beta$ inverse agonists.. <b>2021</b> , 229, 114065	1

157	Polypharmacology: The science of multi-targeting molecules.. <b>2022</b> , 176, 106055	8
156	Advances in structure-based virtual screening for drug discovery. <b>2022</b> , 387-404	
155	2-Aminopyridine - an unsung hero in drug discovery.. <b>2021</b> ,	3
154	Synthesis of Substituted Pyrano[3,4- b ]Quinolines by Silver-Catalyzed Regioselective Intramolecular Cyclization of 3-Alkynylquinoline Aldehydes.	
153	Natural product drug discovery in the artificial intelligence era.. <b>2022</b> , 13, 1526-1546	11
152	Fragment-Based Discovery of MRTX1719, a Synthetic Lethal Inhibitor of the PRMT5MTA Complex for the Treatment of -Deleted Cancers.. <b>2022</b> ,	7
151	Directing Crystallization Outcomes of Conformationally Flexible Molecules: Polymorphs, Solvates, and Desolvation Pathways of Fluconazole.. <b>2022</b> ,	0
150	Screening the Efficacy of Melatonin on Neurodegeneration Mediated by Endoplasmic Reticulum Stress, Inflammation, and Oxidative Damage.. <b>2022</b> , 194, 1105	
149	Properties of FDA-approved small molecule protein kinase inhibitors: a 2022 update.. <b>2021</b> , 106037	22
148	Synthesis of aminoethyl substituted piperidine derivatives as $\mu$ receptor ligands with antiproliferative properties.. <b>2022</b> ,	1
147	Drug-likeness scoring based on unsupervised learning.. <b>2022</b> , 13, 554-565	0
146	to development of a polyherbal against .. <b>2022</b> , 8, e08789	
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144	Synthesis of tropane-based $\mu$ receptor antagonists with antiallodynic activity.. <b>2022</b> , 230, 114113	1
143	Optimization of physicochemical properties is a strategy to improve drug-likeness associated with activity: novel active and selective compounds against Trypanosoma cruzi.. <b>2022</b> , 171, 106114	0
142	Regioselective synthesis, physicochemical properties and anticancer activity of 2-aminomethylated estrone derivatives.. <b>2022</b> , 219, 106064	0
141	Discovery of HDAC6-Selective Inhibitor NN-390 with Efficacy in Group 3 Medulloblastoma.. <b>2022</b> ,	4
140	Selected Applications of Spirocycles in Medicinal Chemistry. <b>2022</b> , 9-34	

139	Machine learning & deep learning in data-driven decision making of drug discovery and challenges in high-quality data acquisition in the pharmaceutical industry.. <b>2021</b> ,	0
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135	Discovery of Novel 3-Piperidinyl Pyridine Derivatives as Highly Potent and Selective Cholesterol 24-Hydroxylase (CH24H) Inhibitors.. <b>2022</b> ,	1
134	Discovery of Brain-Penetrant Glucosylceramide Synthase Inhibitors with a Novel Pharmacophore.. <b>2022</b> ,	1
133	Novel Macrocyclic Antagonists of the Calcitonin Gene-Related Peptide Receptor: Design, Realization, and Structural Characterization of Protein-Ligand Complexes.. <b>2022</b> ,	0
132	Association of Dietary Intake of Polyphenols with an Adequate Nutritional Profile in Postpartum Women from Argentina.. <b>2022</b> , 27, 20-36	1
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129	Covalent Proximity Scanning of a Distal Cysteine to Target PI3Kβ <b>2022</b> ,	4
128	In Silico Approaches for Some Sulfa Drugs as Eco-Friendly Corrosion Inhibitors of Iron in Aqueous Medium. <b>2022</b> , 10, 43	0
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99	Discovery of benzamide derivatives containing urea moiety as soluble epoxide hydrolase inhibitors. <b>2022</b> , 105898	0
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55	Properties of FDA-approved Small Molecule Protein Kinase Inhibitors: A 2023 Update. <b>2022</b> , 106552	6
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53	Insights into the equilibrium structure and translocation mechanism of TP1, a spontaneous membrane-translocating peptide. <b>2022</b> , 12,	0
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41	Integration of Synthetic Organic Chemistry and <i>in silico</i> Drug Discovery - Lead Discovery of Renin Inhibitors and <i>O</i> -GlcNAcase Inhibitors. <b>2023</b> , 81, 25-34	0
40	Fragment-to-Lead Medicinal Chemistry Publications in 2021.	0
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28	Drug discovery: Standing on the shoulders of giants. <b>2023</b> , 207-338	0
27	Systematic Potency and Property Assessment of VHL Ligands and Implications on PROTAC Design.	0
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25	Endocannabinoid Degradation Enzyme Inhibitors as Potential Antipsychotics: A Medicinal Chemistry Perspective. <b>2023</b> , 11, 469	0
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23	Trends in Molecular Properties, Bioavailability, and Permeability across the Bayer Compound Collection. <b>2023</b> , 66, 2347-2360	0
22	Screening for bilayer-active and likely cytotoxic molecules reveals bilayer-mediated regulation of cell function. <b>2023</b> , 155,	0
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