Gerhard Wolber

List of Publications by Year
in descending order

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193	8,645	53660 45	53109 85
papers	citations	h-index	g-index

203	203	203	9994
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	LigandScout:Â 3-D Pharmacophores Derived from Protein-Bound Ligands and Their Use as Virtual Screening Filters. Journal of Chemical Information and Modeling, 2005, 45, 160-169.	2.5	1,576
2	Evaluation of the performance of 3D virtual screening protocols: RMSD comparisons, enrichment assessments, and decoy selectionâ€"What can we learn from earlier mistakes?. Journal of Computer-Aided Molecular Design, 2008, 22, 213-228.	1.3	330
3	Benzimidazol-2-ylidene Gold(I) Complexes Are Thioredoxin Reductase Inhibitors with Multiple Antitumor Properties. Journal of Medicinal Chemistry, 2010, 53, 8608-8618.	2.9	301
4	Molecule-pharmacophore superpositioning and pattern matching in computational drug design. Drug Discovery Today, 2008, 13, 23-29.	3.2	287
5	Efficient overlay of small organic molecules using 3D pharmacophores. Journal of Computer-Aided Molecular Design, 2007, 20, 773-788.	1.3	265
6	How To Optimize Shape-Based Virtual Screening: Choosing the Right Query and Including Chemical Information. Journal of Chemical Information and Modeling, 2009, 49, 678-692.	2.5	178
7	The impact of molecular dynamics on drug design: applications for the characterization of ligandâ€"macromolecule complexes. Drug Discovery Today, 2015, 20, 686-702.	3.2	171
8	Comparative Performance Assessment of the Conformational Model Generators Omega and Catalyst:Â A Large-Scale Survey on the Retrieval of Protein-Bound Ligand Conformations. Journal of Chemical Information and Modeling, 2006, 46, 1848-1861.	2.5	159
9	Comparative Analysis of Protein-Bound Ligand Conformations with Respect to Catalyst's Conformational Space Subsampling Algorithms. Journal of Chemical Information and Modeling, 2005, 45, 422-430.	2.5	148
10	In silicoTarget Fishing for Rationalized Ligand Discovery Exemplified on Constituents ofRuta graveolens. Planta Medica, 2009, 75, 195-204.	0.7	131
11	Next generation 3D pharmacophore modeling. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1468.	6.2	122
12	Antiviral Potential and Molecular Insight into Neuraminidase Inhibiting Diarylheptanoids from Alpinia katsumadai. Journal of Medicinal Chemistry, 2010, 53, 778-786.	2.9	114
13	Design, synthesis and molecular docking study of novel quinoxalin-2(1H)-ones as anti-tumor active agents with inhibition of tyrosine kinase receptor and studying their cyclooxygenase-2 activity. European Journal of Medicinal Chemistry, 2014, 86, 122-132.	2.6	110
14	Strategies for 3D pharmacophore-based virtual screening. Drug Discovery Today: Technologies, 2010, 7, e221-e228.	4.0	97
15	Anthocyanin composition, antioxidant efficiency, and Î±-amylase inhibitor activity of different Hungarian sour cherry varieties (Prunus cerasus L.). Food Chemistry, 2016, 194, 222-229.	4.2	93
16	The Protein Data Bank (PDB), Its Related Services and Software Tools as Key Components for In Silico Guided Drug Discovery. Journal of Medicinal Chemistry, 2008, 51, 7021-7040.	2.9	91
17	The UV-filter benzophenone-1 inhibits 17Î²-hydroxysteroid dehydrogenase type 3: Virtual screening as a strategy to identify potential endocrine disrupting chemicals. Biochemical Pharmacology, 2010, 79, 1189-1199.	2.0	78
18	Enhancing Drug Discovery Through In Silico Screening: Strategies to Increase True Positives Retrieval Rates. Current Medicinal Chemistry, 2008, 15, 2040-2053.	1.2	76

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19	Pharmacophore definition and 3D searches. Drug Discovery Today: Technologies, 2004, 1, 203-207.	4.0	75
20	NSC23766, a Widely Used Inhibitor of Rac1 Activation, Additionally Acts as a Competitive Antagonist at Muscarinic Acetylcholine Receptors. Journal of Pharmacology and Experimental Therapeutics, 2013, 347, 69-79.	1.3	75
21	Ecdysteroids: A novel class of anabolic agents?. Biology of Sport, 2014, 32, 169-173.	1.7	75
22	Computer-Aided Discovery, Validation, and Mechanistic Characterization of Novel Neolignan Activators of Peroxisome Proliferator-Activated Receptor Î³. Molecular Pharmacology, 2010, 77, 559-566.	1.0	72
23	Fast and Efficient in Silico 3D Screening:â€‰ Toward Maximum Computational Efficiency of Pharmacophore-Based and Shape-Based Approaches. Journal of Chemical Information and Modeling, 2007, 47, 2182-2196.	2.5	69
24	Discovery of novel benzene 1,3-dicarboxylic acid inhibitors of bacterial MurD and MurE ligases by structure-based virtual screening approach. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 2668-2673.	1.0	67
25	In silico virtual screening approaches for anti-viral drug discovery. Drug Discovery Today: Technologies, 2012, 9, e219-e225.	4.0	67
26	Ligand Binding Ensembles Determine Graded Agonist Efficacies at a G Protein-coupled Receptor. Journal of Biological Chemistry, 2016, 291, 16375-16389.	1.6	67
27	Discovery of Novel PPAR Ligands by a Virtual Screening Approach Based on Pharmacophore Modeling, 3D Shape, and Electrostatic Similarity Screening. Journal of Medicinal Chemistry, 2008, 51, 6303-6317.	2.9	65
28	Selective Inhibitors of the Protein Tyrosine Phosphatase SHP2 Block Cellular Motility and Growth of Cancer Cells inâ€…vitro and inâ€…vivo. ChemMedChem, 2015, 10, 815-826.	1.6	65
29	Identification of HIV-1 reverse transcriptase dual inhibitors by a combined shape-, 2D-fingerprint- and pharmacophore-based virtual screening approach. European Journal of Medicinal Chemistry, 2012, 50, 216-229.	2.6	63
30	Pharmacophore-based discovery of FXR-agonists. Part II: Identification of bioactive triterpenes from Ganoderma lucidum. Bioorganic and Medicinal Chemistry, 2011, 19, 6779-6791.	1.4	59
31	Identification of Bioactive Natural Products by Pharmacophore-Based Virtual Screening. Current Pharmaceutical Design, 2010, 16, 1666-1681.	0.9	58
32	Novel pharmacological chaperones that correct phenylketonuria in mice. Human Molecular Genetics, 2012, 21, 1877-1887.	1.4	58
33	Characterization of activity and binding mode of glycyrrhetinic acid derivatives inhibiting 11Î²-hydroxysteroid dehydrogenase type 2. Journal of Steroid Biochemistry and Molecular Biology, 2011, 125, 129-142.	1.2	57
34	Legacy data sharing to improve drug safety assessment: the eTOX project. Nature Reviews Drug Discovery, 2017, 16, 811-812.	21.5	56
35	Discovery of Nonsteroidal 17Î²-Hydroxysteroid Dehydrogenase 1 Inhibitors by Pharmacophore-Based Screening of Virtual Compound Libraries. Journal of Medicinal Chemistry, 2008, 51, 4188-4199.	2.9	55
36	The µ Opioid Receptor and Ligands Acting at the µ Opioid Receptor, as Therapeutics and Potential Therapeutics. Current Pharmaceutical Design, 2014, 19, 7415-7434.	0.9	55

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37	One Concept, Three Implementations of 3D Pharmacophore-Based Virtual Screening: Distinct Coverage of Chemical Search Space. Journal of Chemical Information and Modeling, 2010, 50, 1241-1247.	2.5	54
38	Pharmacophore Modeling and Virtual Screening for Novel Acidic Inhibitors of Microsomal Prostaglandin E₂ Synthase-1 (mPGES-1). Journal of Medicinal Chemistry, 2011, 54, 3163-3174.	2.9	53
39	High-throughput structure-based pharmacophore modelling as a basis for successful parallel virtual screening. Journal of Computer-Aided Molecular Design, 2007, 20, 703-715.	1.3	52
40	11Î²-Hydroxysteroid dehydrogenase 1 inhibiting constituents from Eriobotrya japonica revealed by bioactivity-guided isolation and computational approaches. Bioorganic and Medicinal Chemistry, 2010, 18, 1507-1515.	1.4	50
41	Discovery of a novel IKK-Î² inhibitor by ligand-based virtual screening techniques. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 577-583.	1.0	50
42	Identification of PPARgamma Partial Agonists of Natural Origin (I): Development of a Virtual Screening Procedure and In Vitro Validation. PLoS ONE, 2012, 7, e50816.	1.1	48
43	Development of Novel Peptidomimetics Containing a Vinyl Sulfone Moiety as Proteasome Inhibitors. ChemMedChem, 2011, 6, 1228-1237.	1.6	47
44	Synthesis, biological activity and structureâ€“activity relationships of new benzoic acid-based protein tyrosine phosphatase inhibitors endowed with insulinomimetic effects in mouse C2C12 skeletal muscle cells. European Journal of Medicinal Chemistry, 2014, 71, 112-127.	2.6	47
45	Inhibitory potency of flavonoid derivatives on influenza virus neuraminidase. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 4312-4317.	1.0	47
46	Morphinans and isoquinolines: Acetylcholinesterase inhibition, pharmacophore modeling, and interaction with opioid receptors. Bioorganic and Medicinal Chemistry, 2010, 18, 5071-5080.	1.4	46
47	Pharmacophore-based discovery of FXR agonists. Part I: Model development and experimental validation. Bioorganic and Medicinal Chemistry, 2011, 19, 7168-7180.	1.4	46
48	Peptideâ€Based Proteasome Inhibitors in Anticancer Drug Design. Medicinal Research Reviews, 2014, 34, 1001-1069.	5.0	46
49	Selective inhibition of 11Î²-hydroxysteroid dehydrogenase 1 by 18Î±-glycyrrhetinic acid but not 18Î²-glycyrrhetinic acid. Journal of Steroid Biochemistry and Molecular Biology, 2009, 113, 248-252.	1.2	45
50	Computational close up on proteinâ€“protein interactions: how to unravel the invisible using molecular dynamics simulations?. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 345-359.	6.2	45
51	Nâ€methylâ€Dâ€aspartate receptor dysfunction by unmutated human antibodies against the NR1 subunit. Annals of Neurology, 2019, 85, 771-776.	2.8	44
52	Development of Anti-Viral Agents Using Molecular Modeling and Virtual Screening Techniques. Infectious Disorders - Drug Targets, 2011, 11, 64-93.	0.4	43
53	Critical Comparison of Virtual Screening Methods against the MUV Data Set. Journal of Chemical Information and Modeling, 2009, 49, 2168-2178.	2.5	42
54	More than a look into a crystal ball: protein structure elucidation guided by molecular dynamics simulations. Drug Discovery Today, 2016, 21, 1799-1805.	3.2	41

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55	Efficient substrate screening and inhibitor testing of human CYP4Z1 using permeabilized recombinant fission yeast. Biochemical Pharmacology, 2017, 146, 174-187.	2.0	40
56	Design, synthesis and structureâ€“activity relationship of novel quinoxaline derivatives as cancer chemopreventive agent by inhibition of tyrosine kinase receptor. European Journal of Medicinal Chemistry, 2013, 69, 115-124.	2.6	38
57	Discovery of Novel CB₂ Receptor Ligands by a Pharmacophore-Based Virtual Screening Workflow. Journal of Medicinal Chemistry, 2009, 52, 369-378.	2.9	37
58	An investigation on 4-thiazolidinone derivatives as dual inhibitors of aldose reductase and protein tyrosine phosphatase 1B, in the search for potential agents for the treatment of type 2 diabetes mellitus and its complications. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 3712-3720.	1.0	37
59	Virtual combinatorial chemistry and in silico screening: Efficient tools for lead structure discovery?. Pure and Applied Chemistry, 2004, 76, 991-996.	0.9	36
60	Impact of fluorination on proteolytic stability of peptides: a case study with Î±-chymotrypsin and pepsin. Amino Acids, 2014, 46, 2733-2744.	1.2	36
61	Immunoproteasome-Selective Inhibitors: A Promising Strategy to Treat Hematologic Malignancies, Autoimmune and Inflammatory Diseases. Current Medicinal Chemistry, 2016, 23, 1217-1238.	1.2	36
62	Chemoenzymatic Synthesis of Nonasulfated Tetrahyaluronan with a Paramagnetic Tag for Studying Its Complex with Interleukinâ€10. Chemistry - A European Journal, 2016, 22, 5563-5574.	1.7	35
63	New 4-[(5-arylidene-2-arylimino-4-oxo-3-thiazolidinyl)methyl]benzoic acids active as protein tyrosine phosphatase inhibitors endowed with insulinomimetic effect on mouse C2C12 skeletal muscle cells. European Journal of Medicinal Chemistry, 2012, 50, 332-343.	2.6	34
64	Development of peptidomimetic boronates as proteasome inhibitors. European Journal of Medicinal Chemistry, 2013, 64, 23-34.	2.6	34
65	Benzene-1,3-dicarboxylic acid 2,5-dimethylpyrrole derivatives as multiple inhibitors of bacterial Mur ligases (MurCâ€“MurF). Bioorganic and Medicinal Chemistry, 2014, 22, 4124-4134.	1.4	34
66	Binding mechanism investigations guiding the synthesis of novel condensed 1,4-dihydropyridine derivatives with L-/T-type calcium channel blocking activity. European Journal of Medicinal Chemistry, 2018, 155, 1-12.	2.6	34
67	Predicting Cyclooxygenase Inhibition by Threeâ€Dimensional Pharmacophoric Profiling. Part I: Model Generation, Validation and Applicability in Ethnopharmacology. Molecular Informatics, 2010, 29, 75-86.	1.4	33
68	Identification of chemically diverse, novel inhibitors of 17Î²-hydroxysteroid dehydrogenase type 3 and 5 by pharmacophore-based virtual screening. Journal of Steroid Biochemistry and Molecular Biology, 2011, 125, 148-161.	1.2	33
69	Synthesis and biological assessment of novel 2-thiazolylhydrazones and computational analysis of their recognition by monoamine oxidase B. European Journal of Medicinal Chemistry, 2012, 48, 284-295.	2.6	33
70	Prospective Virtual Screening in a Sparse Data Scenario: Design of Smallâ€Molecule TLR2 Antagonists. ChemMedChem, 2014, 9, 813-822.	1.6	33
71	Strategies for the discovery of biased GPCR ligands. Drug Discovery Today, 2019, 24, 1031-1037.	3.2	33
72	Dualsteric Muscarinic Antagonistsâ€“Orthosteric Binding Pose Controls Allosteric Subtype Selectivity. Journal of Medicinal Chemistry, 2014, 57, 6739-6750.	2.9	32

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73	Polyacetylenes from carrots (Daucus carota) improve glucose uptake in vitro in adipocytes and myotubes. Food and Function, 2015, 6, 2135-2144.	2.1	31
74	Fluorination of Photoswitchable Muscarinic Agonists Tunes Receptor Pharmacology and Photochromic Properties. Journal of Medicinal Chemistry, 2019, 62, 3009-3020.	2.9	31
75	Irreversible inhibitors of the 3C protease of Coxsackie virus through templated assembly of protein-binding fragments. Nature Communications, 2016, 7, 12761.	5.8	30
76	Arginase Structure and Inhibition: Catalytic Site Plasticity Reveals New Modulation Possibilities. Scientific Reports, 2017, 7, 13616.	1.6	30
77	Discovery of 4-[(5-arylidene-4-oxothiazolidin-3-yl)methyl]benzoic acid derivatives active as novel potent allosteric inhibitors of protein tyrosine phosphatase 1B: In silico studies and inÂvitro evaluation as insulinomimetic and anti-inflammatory agents. European Journal of Medicinal Chemistry, 2017, 127, 840-858.	2.6	30
78	Design, synthesis, antibacterial activity evaluation and molecular modeling studies of new sulfonamides containing a sulfathiazole moiety. New Journal of Chemistry, 2021, 45, 8166-8177.	1.4	30
79	Butyltin(IV) Benzoates: Inhibition of Thioredoxin Reductase, Tumor Cell Growth Inhibition, and Interactions with Proteins. ChemMedChem, 2013, 8, 256-264.	1.6	27
80	Optimization of peptidomimetic boronates bearing a P3 bicyclic scaffold as proteasome inhibitors. European Journal of Medicinal Chemistry, 2014, 83, 1-14.	2.6	27
81	Selected cytotoxic gold compounds cause significant inhibition of 20S proteasome catalytic activities. Journal of Inorganic Biochemistry, 2014, 141, 79-82.	1.5	27
82	In Silico Prediction of Human Sulfotransferase 1E1 Activity Guided by Pharmacophores from Molecular Dynamics Simulations. Journal of Biological Chemistry, 2016, 291, 58-71.	1.6	27
83	Characterization of new PPARÎ³ agonists: Benzimidazole derivativesâ€"importance of positions 5 and 6, and computational studies on the binding mode. Bioorganic and Medicinal Chemistry, 2010, 18, 5885-5895.	1.4	26
84	Balancing Inflammation: Computational Design of Small-Molecule Toll-like Receptor Modulators. Trends in Pharmacological Sciences, 2017, 38, 155-168.	4.0	26
85	Discovery of Novel Cathepsin S Inhibitors by Pharmacophore-Based Virtual High-Throughput Screening. Journal of Chemical Information and Modeling, 2008, 48, 1693-1705.	2.5	25
86	Computational Tools for In Silico Fragment-Based Drug Design. Current Topics in Medicinal Chemistry, 2012, 12, 1935-1943.	1.0	25
87	Molecular dynamics simulation and linear interaction energy study of d-Glu-based inhibitors of the MurD ligase. Journal of Computer-Aided Molecular Design, 2013, 27, 723-738.	1.3	25
88	Identification of a new series of amides as non-covalent proteasome inhibitors. European Journal of Medicinal Chemistry, 2014, 76, 1-9.	2.6	25
89	Isolation of a Novel Thioflavin Sâ€"Derived Compound That Inhibits BAG-1â€"Mediated Protein Interactions and Targets BRAF Inhibitorâ€"Resistant Cell Lines. Molecular Cancer Therapeutics, 2013, 12, 2400-2414.	1.9	23
90	Structure versus functionâ€"The impact of computational methods on the discovery of specific GPCRâ€"ligands. Bioorganic and Medicinal Chemistry, 2015, 23, 3907-3912.	1.4	23

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91	Molecular insight on the binding of NNRTI to K103N mutated HIV-1 RT: molecular dynamics simulations and dynamic pharmacophore analysis. Molecular BioSystems, 2016, 12, 3385-3395.	2.9	23
92	Acute myeloid leukaemia-derived Langerhans-like cells enhance Th1 polarization upon TLR2 engagement. Pharmacological Research, 2016, 105, 44-53.	3.1	23
93	Ligand-Specific Restriction of Extracellular Conformational Dynamics Constrains Signaling of the M₂ Muscarinic Receptor. ACS Chemical Biology, 2017, 12, 1743-1748.	1.6	23
94	Structural Characteristics of the Allosteric Binding Site Represent a Key to Subtype Selective Modulators of Muscarinic Acetylcholine Receptors. Molecular Informatics, 2015, 34, 526-530.	1.4	22
95	New telmisartan-derived PPARÎ³ agonists: Impact of the 3D-binding mode on the pharmacological profile. European Journal of Medicinal Chemistry, 2016, 124, 138-152.	2.6	22
96	Inhibitor Design Strategy Based on an Enzyme Structural Flexibility: A Case of Bacterial MurD Ligase. Journal of Chemical Information and Modeling, 2014, 54, 1451-1466.	2.5	21
97	Furan-based benzene mono- and dicarboxylic acid derivatives as multiple inhibitors of the bacterial Mur ligases (MurCâ€“MurF): experimental and computational characterization. Journal of Computer-Aided Molecular Design, 2015, 29, 541-560.	1.3	21
98	Identification of noncovalent proteasome inhibitors with high selectivity for chymotrypsin-like activity by a multistep structure-based virtual screening. European Journal of Medicinal Chemistry, 2016, 121, 578-591.	2.6	21
99	The novel small-molecule antagonist MMG-11 preferentially inhibits TLR2/1 signaling. Biochemical Pharmacology, 2020, 171, 113687.	2.0	21
100	Natural Products in Structure-Assisted Design of Molecular Cancer Therapeutics. Current Pharmaceutical Design, 2010, 16, 1718-1741.	0.9	20
101	Optimization of the N-Lost Drugs Melphalan and Bendamustine: Synthesis and Cytotoxicity of a New Set of Dendrimerâ"Drug Conjugates as Tumor Therapeutic Agents. Bioconjugate Chemistry, 2010, 21, 1728-1743.	1.8	20
102	Combined chemical and biotechnological production of 20Î²OH-NorDHCMT, a long-term metabolite of Oral-Turinabol (DHCMT). Journal of Inorganic Biochemistry, 2018, 183, 165-171.	1.5	20
103	Phenylthiomethyl Ketone-Based Fragments Show Selective and Irreversible Inhibition of Enteroviral 3C Proteases. Journal of Medicinal Chemistry, 2018, 61, 1218-1230.	2.9	20
104	Identification of a pyrogallol derivative as a potent and selective human TLR2 antagonist by structure-based virtual screening. Biochemical Pharmacology, 2018, 154, 148-160.	2.0	20
105	3D-QSAR, design, synthesis and characterization of trisubstituted harmine derivatives with inÂvitro antiproliferative properties. European Journal of Medicinal Chemistry, 2015, 94, 45-55.	2.6	19
106	Structural insights into understudied human cytochrome P450 enzymes. Drug Discovery Today, 2021, 26, 2456-2464.	3.2	19
107	Applications of Integrated Data Mining Methods to Exploring Natural Product Space for Acetylcholinesterase Inhibitors. Combinatorial Chemistry and High Throughput Screening, 2010, 13, 54-66.	0.6	18
108	Isomeric C12-Alkamides from the Roots of Echinacea purpurea Improve Basal and Insulin-Dependent Glucose Uptake in 3T3-L1 Adipocytes. Planta Medica, 2014, 80, 1712-1720.	0.7	18

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109	From carbohydrates to drug-like fragments: Rational development of novel Î±-amylase inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 6725-6732.	1.4	18
110	Functional characterization and mechanistic modeling of the human cytochrome P450 enzyme CYP4A22. FEBS Letters, 2019, 593, 2214-2225.	1.3	18
111	HuskinDB, a database for skin permeation of xenobiotics. Scientific Data, 2020, 7, 426.	2.4	18
112	Influence of Chlorine or Fluorine Substitution on the Estrogenic Properties of 1-Alkyl-2,3,5-tris(4-hydroxyphenyl)-1H-pyrroles. Journal of Medicinal Chemistry, 2012, 55, 9607-9618.	2.9	17
113	Design, synthesis, inhibition studies, and molecular modeling of pepstatin analogues addressing different secreted aspartic proteinases of Candida albicans. Biochemical Pharmacology, 2013, 85, 881-887.	2.0	17
114	Identification of PPARÎ³ Agonists from Natural Sources Using Different In Silico Approaches. Planta Medica, 2015, 81, 488-494.	0.7	17
115	Enhanced immunostimulatory activity of in silico discovered agonists of Toll-like receptor 2 (TLR2). Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 2680-2689.	1.1	17
116	Importance of asparagine-381 and arginine-487 for substrate recognition in CYP4Z1. Biochemical Pharmacology, 2020, 174, 113850.	2.0	17
117	Identification of Novel Liver X Receptor Activators by Structure-Based Modeling. Journal of Chemical Information and Modeling, 2012, 52, 1391-1400.	2.5	16
118	Development of Novel Selective Peptidomimetics Containing a Boronic Acid Moiety, Targeting the 20S Proteasome as Anticancer Agents. ChemMedChem, 2014, 9, 1801-1816.	1.6	16
119	Discovery of Michael acceptor containing 1,4-dihydropyridines as first covalent inhibitors of L-/T-type calcium channels. Bioorganic Chemistry, 2019, 91, 103187.	2.0	16
120	PyRod: Tracing Water Molecules in Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2019, 59, 2818-2829.	2.5	16
121	Ligand-guided homology modeling drives identification of novel histamine H3 receptor ligands. PLoS ONE, 2019, 14, e0218820.	1.1	16
122	In Search for Multi-Target Ligands as Potential Agents for Diabetes Mellitus and Its Complicationsâ€"A Structure-Activity Relationship Study on Inhibitors of Aldose Reductase and Protein Tyrosine Phosphatase 1B. Molecules, 2021, 26, 330.	1.7	16
123	Predicting cyclooxygenase inhibition by three-dimensional pharmacophoric profiling. Part II: Identification of enzyme inhibitors from Prasaplai, a Thai traditional medicine. Phytomedicine, 2011, 18, 119-133.	2.3	15
124	Interruption of the Ionic Lock in the Bradykinin B₂ Receptor Results in Constitutive Internalization and Turns Several Antagonists into Strong Agonists. Journal of Pharmacology and Experimental Therapeutics, 2013, 344, 85-95.	1.3	15
125	Synthesis, Biological Evaluation, and Docking Studies of New 2â€Furylbenzimidazoles as Antiâ€Angiogenic Agents: Part II. Archiv Der Pharmazie, 2014, 347, 291-304.	2.1	15
126	Ligand-Specific Allosteric Coupling Controls G-Protein-Coupled Receptor Signaling. ACS Pharmacology and Translational Science, 2020, 3, 859-867.	2.5	15

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127	Design and evaluation of non-carboxylate 5-arylidene-2-thioxo-4-imidazolidinones as novel non-competitive inhibitors of protein tyrosine phosphatase 1B. Bioorganic Chemistry, 2019, 92, 103211.	2.0	14
128	Fine-mapping of the substrate specificity of human steroid 21-hydroxylase (CYP21A2). Journal of Steroid Biochemistry and Molecular Biology, 2019, 194, 105446.	1.2	14
129	Mechanistic Understanding of Peptide Analogues, DALDA, [Dmt1]DALDA, and KGOP01, Binding to the Mu Opioid Receptor. Molecules, 2020, 25, 2087.	1.7	14
130	N-Phenethyl Substitution in 14-Methoxy-N-methylmorphinan-6-ones Turns Selective Âμ Opioid Receptor Ligands into Dual Âμ/Î´ Opioid Receptor Agonists. Scientific Reports, 2020, 10, 5653.	1.6	14
131	Pharmacophore-based discovery of a novel cytosolic phospholipase A2Î± inhibitor. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 1202-1207.	1.0	13
132	Discovery of a novel potent cytochrome P450 CYP4Z1 inhibitor. European Journal of Medicinal Chemistry, 2021, 215, 113255.	2.6	13
133	Synthesis, crystallographic characterization, molecular docking and biological activity of isoquinoline derivatives. Chemistry Central Journal, 2017, 11, 103.	2.6	12
134	Current κ Opioid Receptor Ligands and Discovery of a New Molecular Scaffold as a κ Opioid Receptor Antagonist Using Pharmacophore-Based Virtual Screening. Current Pharmaceutical Design, 2014, 19, 7362-7372.	0.9	12
135	Functional Expression of All Human Sulfotransferases in Fission Yeast, Assay Development, and Structural Models for Isoforms SULT4A1 and SULT6B1. Biomolecules, 2020, 10, 1517.	1.8	11
136	Design and synthesis of 3,5-substituted 1,2,4-oxadiazoles as catalytic inhibitors of human DNA topoisomerase IIÎ±. Bioorganic Chemistry, 2020, 99, 103828.	2.0	11
137	An Unusual Interstrand H-Bond Stabilizes the Heteroassembly of Helical Î±Î²Î³-Chimeras with Natural Peptides. ACS Chemical Biology, 2014, 9, 613-616.	1.6	10
138	A common polymorphic variant of <scp>UGT</scp>1A5 displays increased activity due to optimized cofactor binding. FEBS Letters, 2018, 592, 1837-1846.	1.3	10
139	Identification and characterization of a novel chemotype for human TLR8 inhibitors. European Journal of Medicinal Chemistry, 2019, 179, 744-752.	2.6	10
140	Catching a Moving Target: Comparative Modeling of Flaviviral NS2B-NS3 Reveals Small Molecule Zika Protease Inhibitors. ACS Medicinal Chemistry Letters, 2020, 11, 514-520.	1.3	10
141	3D pharmacophore elucidation and virtual screening. Drug Discovery Today: Technologies, 2010, 7, e203-e204.	4.0	9
142	Binding characteristics of [³H]â€‰SM10292: a new cell membraneâ€permeant nonâ€peptide bradykinin B₂ receptor antagonist. British Journal of Pharmacology, 2012, 167, 839-853.	2.7	9
143	New Proluciferin Substrates for Human CYP4 Family Enzymes. Applied Biochemistry and Biotechnology, 2021, 193, 218-237.	1.4	9
144	Antinociceptive Efficacy of the Âμ-Opioid/Nociceptin Peptide-Based Hybrid KGNOP1 in Inflammatory Pain without Rewarding Effects in Mice: An Experimental Assessment and Molecular Docking. Molecules, 2021, 26, 3267.	1.7	9

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145	Chemical Evolution of Antivirals Against Enterovirus D68 through Proteinâ€Templated Knoevenagel Reactions. Angewandte Chemie - International Edition, 2021, 60, 13294-13301.	7.2	9
146	In silico discovery of acylated flavonol monorhamnosides from Eriobotrya japonica as natural, small-molecular weight inhibitors of XIAP BIR3. Bioorganic and Medicinal Chemistry, 2011, 19, 1002-1009.	1.4	8
147	Î²- and Î³-Amino Acids at Î±-Helical Interfaces: Toward the Formation of Highly Stable Foldameric Coiled Coils. ACS Medicinal Chemistry Letters, 2014, 5, 1300-1303.	1.3	8
148	Discovery of Sanggenon G as a natural cellâ€permeable smallâ€molecular weight inhibitor of Xâ€linked inhibitor of apoptosis protein (XIAP). FEBS Open Bio, 2014, 4, 659-671.	1.0	8
149	Structural determinants of diphenethylamines for interaction with the Îº opioid receptor: Synthesis, pharmacology and molecular modeling studies. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 4769-4774.	1.0	8
150	Identification of 2-thioxoimidazolidin-4-one derivatives as novel noncovalent proteasome and immunoproteasome inhibitors. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 278-283.	1.0	8
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