Gerhard Wolber

List of Publications by Citations

192 papers	6,950 citations	42 h-index	76 g-index
203 ext. papers	7,934 ext. citations	5.5 avg, IF	6.01 L-index

#	Paper	IF	Citations
192	LigandScout: 3-D pharmacophores derived from protein-bound ligands and their use as virtual screening filters. *Journal of Chemical Information and Modeling*, **2005**, 45, 160-9	6.1	1255
191	Evaluation of the performance of 3D virtual screening protocols: RMSD comparisons, enrichment assessments, and decoy selection--what can we learn from earlier mistakes?. *Journal of Computer-Aided Molecular Design*, **2008**, 22, 213-28	4.2	278
190	Benzimidazol-2-ylidene gold(I) complexes are thioredoxin reductase inhibitors with multiple antitumor properties. *Journal of Medicinal Chemistry*, **2010**, 53, 8608-18	8.3	262
189	Molecule-pharmacophore superpositioning and pattern matching in computational drug design. *Drug Discovery Today*, **2008**, 13, 23-9	8.8	249
188	Efficient overlay of small organic molecules using 3D pharmacophores. *Journal of Computer-Aided Molecular Design*, **2006**, 20, 773-88	4.2	211
187	How to optimize shape-based virtual screening: choosing the right query and including chemical information. *Journal of Chemical Information and Modeling*, **2009**, 49, 678-92	6.1	164
186	Comparative performance assessment of the conformational model generators omega and catalyst: a large-scale survey on the retrieval of protein-bound ligand conformations. *Journal of Chemical Information and Modeling*, **2006**, 46, 1848-61	6.1	151
185	The impact of molecular dynamics on drug design: applications for the characterization of ligand-macromolecule complexes. *Drug Discovery Today*, **2015**, 20, 686-702	8.8	135
184	Comparative analysis of protein-bound ligand conformations with respect to catalyst's conformational space subsampling algorithms. *Journal of Chemical Information and Modeling*, **2005**, 45, 422-30	6.1	125
183	In silico target fishing for rationalized ligand discovery exemplified on constituents of Ruta graveolens. *Planta Medica*, **2009**, 75, 195-204	3.1	111
182	Antiviral potential and molecular insight into neuraminidase inhibiting diarylheptanoids from Alpinia katsumadai. *Journal of Medicinal Chemistry*, **2010**, 53, 778-86	8.3	101
181	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, 7021-40	8.3	81
180	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, 122-32	6.8	78
179	Using structure- and Ligand-based pharmacophores as filters to discriminate Human Aryl Sulfotransferase 1A1 (SUL1A1) binders into substrates and inhibitors. *Journal of Cheminformatics*, **2014**, 6,	8.6	78
178	Efficient 3D pharmacophore alignment as a tool for structure-based modeling and scoring. *Chemistry Central Journal*, **2008**, 2,		78
177	Enhancing drug discovery through in silico screening: strategies to increase true positives retrieval rates. *Current Medicinal Chemistry*, **2008**, 15, 2040-53	4.3	72
176	Anthocyanin composition, antioxidant efficiency, and □-amylase inhibitor activity of different Hungarian sour cherry varieties (Prunus cerasus L.). *Food Chemistry*, **2016**, 194, 222-9	8.5	69

175	Strategies for 3D pharmacophore-based virtual screening. *Drug Discovery Today: Technologies*, **2010**, 7, e203-70	7.1	68
174	Computer-aided discovery, validation, and mechanistic characterization of novel neolignan activators of peroxisome proliferator-activated receptor gamma. *Molecular Pharmacology*, **2010**, 77, 559-66	4.3	66
173	Fast and efficient in silico 3D screening: toward maximum computational efficiency of pharmacophore-based and shape-based approaches. *Journal of Chemical Information and Modeling*, **2007**, 47, 2182-96	6.1	64
172	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, 2668-73	2.9	61
171	The UV-filter benzophenone-1 inhibits 17beta-hydroxysteroid dehydrogenase type 3: Virtual screening as a strategy to identify potential endocrine disrupting chemicals. *Biochemical Pharmacology*, **2010**, 79, 1189-99	6	61
170	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, 6303-17	8.3	60
169	Pharmacophore definition and 3D searches. *Drug Discovery Today: Technologies*, **2004**, 1, 203-7	7.1	59
168	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, 216-29	6.8	55
167	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	4.7	54
166	Characterization of activity and binding mode of glycyrrhetinic acid derivatives inhibiting 11β-hydroxysteroid dehydrogenase type 2. *Journal of Steroid Biochemistry and Molecular Biology*, **2011**, 125, 129-42	5.1	52
165	Selective inhibitors of the protein tyrosine phosphatase SHP2 block cellular motility and growth of cancer cells in vitro and in vivo. *ChemMedChem*, **2015**, 10, 815-26	3.7	51
164	Discovery of nonsteroidal 17beta-hydroxysteroid dehydrogenase 1 inhibitors by pharmacophore-based screening of virtual compound libraries. *Journal of Medicinal Chemistry*, **2008**, 51, 4188-99	8.3	51
163	Ligand Binding Ensembles Determine Graded Agonist Efficacies at a G Protein-coupled Receptor. *Journal of Biological Chemistry*, **2016**, 291, 16375-89	5.4	50
162	Novel pharmacological chaperones that correct phenylketonuria in mice. *Human Molecular Genetics*, **2012**, 21, 1877-87	5.6	50
161	Next generation 3D pharmacophore modeling. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1468	7.9	49
160	Identification of bioactive natural products by pharmacophore-based virtual screening. *Current Pharmaceutical Design*, **2010**, 16, 1666-81	3.3	49
159	Pharmacophore modeling and virtual screening for novel acidic inhibitors of microsomal prostaglandin E-synthase-1 (mPGES-1). *Journal of Medicinal Chemistry*, **2011**, 54, 3163-74	8.3	48
158	Pharmacophore-based discovery of FXR-agonists. Part II: identification of bioactive triterpenes from Ganoderma lucidum. *Bioorganic and Medicinal Chemistry*, **2011**, 19, 6779-91	3.4	48

157	High-throughput structure-based pharmacophore modelling as a basis for successful parallel virtual screening. *Journal of Computer-Aided Molecular Design*, **2006**, 20, 703-15	4.2	47
156	One concept, three implementations of 3D pharmacophore-based virtual screening: distinct coverage of chemical search space. *Journal of Chemical Information and Modeling*, **2010**, 50, 1241-7	6.1	46
155	Ecdysteroids: A novel class of anabolic agents?. *Biology of Sport*, **2015**, 32, 169-73	4.3	45
154	The μ opioid receptor and ligands acting at the μ opioid receptor, as therapeutics and potential therapeutics. *Current Pharmaceutical Design*, **2013**, 19, 7415-34	3.3	44
153	In silico virtual screening approaches for anti-viral drug discovery. *Drug Discovery Today: Technologies*, **2012**, 9, e219-25	7.1	44
152	Pharmacophore-based discovery of FXR agonists. Part I: Model development and experimental validation. *Bioorganic and Medicinal Chemistry*, **2011**, 19, 7168-80	3.4	43
151	Discovery of a novel IKK-β inhibitor by ligand-based virtual screening techniques. *Bioorganic and Medicinal Chemistry Letters*, **2011**, 21, 577-83	2.9	42
150	11beta-Hydroxysteroid dehydrogenase 1 inhibiting constituents from Eriobotrya japonica revealed by bioactivity-guided isolation and computational approaches. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 1507-15	3.4	42
149	Peptide-based proteasome inhibitors in anticancer drug design. *Medicinal Research Reviews*, **2014**, 34, 1001-69	14.4	40
148	Synthesis, biological activity and structure-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, 112-27	6.8	40
147	Morphinans and isoquinolines: acetylcholinesterase inhibition, pharmacophore modeling, and interaction with opioid receptors. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 5071-80	3.4	40
146	Identification of PPARgamma partial agonists of natural origin (I): development of a virtual screening procedure and in vitro validation. *PLoS ONE*, **2012**, 7, e50816	3.7	38
145	Development of novel peptidomimetics containing a vinyl sulfone moiety as proteasome inhibitors. *ChemMedChem*, **2011**, 6, 1228-37	3.7	38
144	Critical comparison of virtual screening methods against the MUV data set. *Journal of Chemical Information and Modeling*, **2009**, 49, 2168-78	6.1	38
143	Legacy data sharing to improve drug safety assessment: the eTOX project. *Nature Reviews Drug Discovery*, **2017**, 16, 811-812	64.1	37
142	More than a look into a crystal ball: protein structure elucidation guided by molecular dynamics simulations. *Drug Discovery Today*, **2016**, 21, 1799-1805	8.8	37
141	Selective inhibition of 11beta-hydroxysteroid dehydrogenase 1 by 18alpha-glycyrrhetinic acid but not 18beta-glycyrrhetinic acid. *Journal of Steroid Biochemistry and Molecular Biology*, **2009**, 113, 248-52	5.1	36
140	Inhibitory potency of flavonoid derivatives on influenza virus neuraminidase. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 4312-7	2.9	34

139	Development of anti-viral agents using molecular modeling and virtual screening techniques. *Infectious Disorders - Drug Targets*, **2011**, 11, 64-93	1.1	33
138	Virtual combinatorial chemistry and in silico screening: Efficient tools for lead structure discovery?. *Pure and Applied Chemistry*, **2004**, 76, 991-996	2.1	33
137	Design, synthesis and structure-activity relationship of novel quinoxaline derivatives as cancer chemopreventive agent by inhibition of tyrosine kinase receptor. *European Journal of Medicinal Chemistry*, **2013**, 69, 115-24	6.8	32
136	Development of peptidomimetic boronates as proteasome inhibitors. *European Journal of Medicinal Chemistry*, **2013**, 64, 23-34	6.8	31
135	Identification of chemically diverse, novel inhibitors of 17β-hydroxysteroid dehydrogenase type 3 and 5 by pharmacophore-based virtual screening. *Journal of Steroid Biochemistry and Molecular Biology*, **2011**, 125, 148-61	5.1	30
134	Discovery of novel CB2 receptor ligands by a pharmacophore-based virtual screening workflow. *Journal of Medicinal Chemistry*, **2009**, 52, 369-78	8.3	30
133	Efficient substrate screening and inhibitor testing of human CYP4Z1 using permeabilized recombinant fission yeast. *Biochemical Pharmacology*, **2017**, 146, 174-187	6	29
132	N-methyl-D-aspartate receptor dysfunction by unmutated human antibodies against the NR1 subunit. *Annals of Neurology*, **2019**, 85, 771-776	9.4	29
131	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, 284-95	6.8	29
130	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, 332-43	6.8	29
129	Chemoenzymatic Synthesis of Nonasulfated Tetrahyaluronan with a Paramagnetic Tag for Studying Its Complex with Interleukin-10. *Chemistry - A European Journal*, **2016**, 22, 5563-74	4.8	29
128	Impact of fluorination on proteolytic stability of peptides: a case study with α-chymotrypsin and pepsin. *Amino Acids*, **2014**, 46, 2733-44	3.5	28
127	Immunoproteasome-Selective Inhibitors: A Promising Strategy to Treat Hematologic Malignancies, Autoimmune and Inflammatory Diseases. *Current Medicinal Chemistry*, **2016**, 23, 1217-38	4.3	27
126	Prospective virtual screening in a sparse data scenario: design of small-molecule TLR2 antagonists. *ChemMedChem*, **2014**, 9, 813-22	3.7	27
125	Benzene-1,3-dicarboxylic acid 2,5-dimethylpyrrole derivatives as multiple inhibitors of bacterial Mur ligases (MurC-MurF). *Bioorganic and Medicinal Chemistry*, **2014**, 22, 4124-34	3.4	27
124	Computational close up on protein–protein interactions: how to unravel the invisible using molecular dynamics simulations?. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2015**, 5, 345-359	7.9	27
123	Predicting Cyclooxygenase Inhibition by Three-Dimensional Pharmacophoric Profiling. Part I: Model Generation, Validation and Applicability in Ethnopharmacology. *Molecular Informatics*, **2010**, 29, 75-86	3.8	27
122	Characterization of new PPARgamma agonists: benzimidazole derivatives-importance of positions 5 and 6, and computational studies on the binding mode. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 5885-95	3.4	26

121	Dualsteric muscarinic antagonists--orthosteric binding pose controls allosteric subtype selectivity. *Journal of Medicinal Chemistry*, **2014**, 57, 6739-50	8.3	25
120	Polyacetylenes from carrots (Daucus carota) improve glucose uptake in vitro in adipocytes and myotubes. *Food and Function*, **2015**, 6, 2135-44	6.1	24
119	Butyltin(IV) benzoates: inhibition of thioredoxin reductase, tumor cell growth inhibition, and interactions with proteins. *ChemMedChem*, **2013**, 8, 256-64	3.7	23
118	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 in vitro evaluation as insulinomimetic and anti-inflammatory agents. *European Journal of Medicinal Chemistry*, **2017**, 127, 840-858	6.8	23
117	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, 723-38	4.2	23
116	Discovery of novel cathepsin S inhibitors by pharmacophore-based virtual high-throughput screening. *Journal of Chemical Information and Modeling*, **2008**, 48, 1693-705	6.1	23
115	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	6.8	23
114	Strategies for the discovery of biased GPCR ligands. *Drug Discovery Today*, **2019**, 24, 1031-1037	8.8	22
113	Irreversible inhibitors of the 3C protease of Coxsackie virus through templated assembly of protein-binding fragments. *Nature Communications*, **2016**, 7, 12761	17.4	22
112	Optimization of peptidomimetic boronates bearing a P3 bicyclic scaffold as proteasome inhibitors. *European Journal of Medicinal Chemistry*, **2014**, 83, 1-14	6.8	22
111	Selected cytotoxic gold compounds cause significant inhibition of 20S proteasome catalytic activities. *Journal of Inorganic Biochemistry*, **2014**, 141, 79-82	4.2	22
110	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	2.9	22
109	Arginase Structure and Inhibition: Catalytic Site Plasticity Reveals New Modulation Possibilities. *Scientific Reports*, **2017**, 7, 13616	4.9	21
108	Structure versus function-The impact of computational methods on the discovery of specific GPCR-ligands. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 3907-12	3.4	21
107	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		21
106	In Silico Prediction of Human Sulfotransferase 1E1 Activity Guided by Pharmacophores from Molecular Dynamics Simulations. *Journal of Biological Chemistry*, **2016**, 291, 58-71	5.4	21
105	Balancing Inflammation: Computational Design of Small-Molecule Toll-like Receptor Modulators. *Trends in Pharmacological Sciences*, **2017**, 38, 155-168	13.2	21
104	Identification of a new series of amides as non-covalent proteasome inhibitors. *European Journal of Medicinal Chemistry*, **2014**, 76, 1-9	6.8	20

103	Computational tools for in silico fragment-based drug design. *Current Topics in Medicinal Chemistry*, **2012**, 12, 1935-43	3	20
102	Pharmacophores from Macromolecular Complexes with LigandScout. *Methods and Principles in Medicinal Chemistry*, **2006**, 131-150	0.4	20
101	Structural Characteristics of the Allosteric Binding Site Represent a Key to Subtype Selective Modulators of Muscarinic Acetylcholine Receptors. *Molecular Informatics*, **2015**, 34, 526-30	3.8	19
100	Ligand-Specific Restriction of Extracellular Conformational Dynamics Constrains Signaling of the M Muscarinic Receptor. *ACS Chemical Biology*, **2017**, 12, 1743-1748	4.9	18
99	Furan-based benzene mono- and dicarboxylic acid derivatives as multiple inhibitors of the bacterial Mur ligases (MurC-MurF): experimental and computational characterization. *Journal of Computer-Aided Molecular Design*, **2015**, 29, 541-60	4.2	18
98	Combined chemical and biotechnological production of 20□H-NorDHCMT, a long-term metabolite of Oral-Turinabol (DHCMT). *Journal of Inorganic Biochemistry*, **2018**, 183, 165-171	4.2	18
97	Acute myeloid leukaemia-derived Langerhans-like cells enhance Th1 polarization upon TLR2 engagement. *Pharmacological Research*, **2016**, 105, 44-53	10.2	18
96	Isolation of a novel thioflavin S-derived compound that inhibits BAG-1-mediated protein interactions and targets BRAF inhibitor-resistant cell lines. *Molecular Cancer Therapeutics*, **2013**, 12, 2400-14	6.1	18
95	Optimization of the N-lost drugs melphalan and bendamustine: synthesis and cytotoxicity of a new set of dendrimer-drug conjugates as tumor therapeutic agents. *Bioconjugate Chemistry*, **2010**, 21, 1728-43	6.3	18
94	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	6.8	18
93	Inhibitor design strategy based on an enzyme structural flexibility: a case of bacterial MurD ligase. *Journal of Chemical Information and Modeling*, **2014**, 54, 1451-66	6.1	17
92	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, 9607-18	8.3	17
91	New telmisartan-derived PPAR□agonists: Impact of the 3D-binding mode on the pharmacological profile. *European Journal of Medicinal Chemistry*, **2016**, 124, 138-152	6.8	17
90	3D-QSAR, design, synthesis and characterization of trisubstituted harmine derivatives with in vitro antiproliferative properties. *European Journal of Medicinal Chemistry*, **2015**, 94, 45-55	6.8	16
89	From carbohydrates to drug-like fragments: Rational development of novel □amylase inhibitors. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 6725-32	3.4	16
88	Natural products in structure-assisted design of molecular cancer therapeutics. *Current Pharmaceutical Design*, **2010**, 16, 1718-41	3.3	16
87	Applications of integrated data mining methods to exploring natural product space for acetylcholinesterase inhibitors. *Combinatorial Chemistry and High Throughput Screening*, **2010**, 13, 54-66	1.3	16
86	Identification of PPAR□Agonists from Natural Sources Using Different In Silico Approaches. *Planta Medica*, **2015**, 81, 488-94	3.1	15

85	Fluorination of Photoswitchable Muscarinic Agonists Tunes Receptor Pharmacology and Photochromic Properties. *Journal of Medicinal Chemistry*, **2019**, 62, 3009-3020	8.3	14
84	Phenylthiomethyl Ketone-Based Fragments Show Selective and Irreversible Inhibition of Enteroviral 3C Proteases. *Journal of Medicinal Chemistry*, **2018**, 61, 1218-1230	8.3	14
83	Design, synthesis, inhibition studies, and molecular modeling of pepstatin analogues addressing different secreted aspartic proteinases of Candida albicans. *Biochemical Pharmacology*, **2013**, 85, 881-7	6	14
82	Enhanced immunostimulatory activity of in silico discovered agonists of Toll-like receptor 2 (TLR2). *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 2680-2689	4	14
81	Functional characterization and mechanistic modeling of the human cytochrome P450 enzyme CYP4A22. *FEBS Letters*, **2019**, 593, 2214-2225	3.8	13
80	Identification of a pyrogallol derivative as a potent and selective human TLR2 antagonist by structure-based virtual screening. *Biochemical Pharmacology*, **2018**, 154, 148-160	6	13
79	Synthesis, biological evaluation, and docking studies of new 2-furylbenzimidazoles as anti-angiogenic agents: part II. *Archiv Der Pharmazie*, **2014**, 347, 291-304	4.3	13
78	Development of novel selective peptidomimetics containing a boronic acid moiety, targeting the 20S proteasome as anticancer agents. *ChemMedChem*, **2014**, 9, 1801-16	3.7	13
77	Identification of novel liver X receptor activators by structure-based modeling. *Journal of Chemical Information and Modeling*, **2012**, 52, 1391-400	6.1	13
76	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	4.7	13
75	Predicting cyclooxygenase inhibition by three-dimensional pharmacophoric profiling. Part II: Identification of enzyme inhibitors from Prasaplai, a Thai traditional medicine. *Phytomedicine*, **2011**, 18, 119-33	6.5	13
74	Ligand-guided homology modeling drives identification of novel histamine H3 receptor ligands. *PLoS ONE*, **2019**, 14, e0218820	3.7	12
73	Importance of asparagine-381 and arginine-487 for substrate recognition in CYP4Z1. *Biochemical Pharmacology*, **2020**, 174, 113850	6	12
72	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*, **2013**, 19, 7362-72	3.3	12
71	The novel small-molecule antagonist MMG-11 preferentially inhibits TLR2/1 signaling. *Biochemical Pharmacology*, **2020**, 171, 113687	6	11
70	Fine-mapping of the substrate specificity of human steroid 21-hydroxylase (CYP21A2). *Journal of Steroid Biochemistry and Molecular Biology*, **2019**, 194, 105446	5.1	10
69	Ligand-Specific Allosteric Coupling Controls G-Protein-Coupled Receptor Signaling. *ACS Pharmacology and Translational Science*, **2020**, 3, 859-867	5.9	10
68	PyRod: Tracing Water Molecules in Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2019**, 59, 2818-2829	6.1	9

67	Mechanistic Understanding of Peptide Analogues, DALDA, [Dmt]DALDA, and KGOP01, Binding to the mu Opioid Receptor. *Molecules*, **2020**, 25,	4.8	9
66	An unusual interstrand H-bond stabilizes the heteroassembly of helical □-chimeras with natural peptides. *ACS Chemical Biology*, **2014**, 9, 613-6	4.9	9
65	Pharmacophore-based discovery of a novel cytosolic phospholipase A(2)□-inhibitor. *Bioorganic and Medicinal Chemistry Letters*, **2012**, 22, 1202-7	2.9	9
64	Isomeric C12-alkamides from the roots of Echinacea purpurea improve basal and insulin-dependent glucose uptake in 3T3-L1 adipocytes. *Planta Medica*, **2014**, 80, 1712-20	3.1	9
63	Binding characteristics of [3H]-JSM10292: a new cell membrane-permeant non-peptide bradykinin B2 receptor antagonist. *British Journal of Pharmacology*, **2012**, 167, 839-53	8.6	9
62	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	5.1	8
61	Catching a Moving Target: Comparative Modeling of Flaviviral NS2B-NS3 Reveals Small Molecule Zika Protease Inhibitors. *ACS Medicinal Chemistry Letters*, **2020**, 11, 514-520	4.3	8
60	Synthesis, crystallographic characterization, molecular docking and biological activity of isoquinoline derivatives. *Chemistry Central Journal*, **2017**, 11, 103		8
59	□-and □-Amino Acids at □-Helical Interfaces: Toward the Formation of Highly Stable Foldameric Coiled Coils. *ACS Medicinal Chemistry Letters*, **2014**, 5, 1300-3	4.3	8
58	3D pharmacophore elucidation and virtual screening. *Drug Discovery Today: Technologies*, **2010**, 7, e203-701		8
57	Discovery of a novel potent cytochrome P450 CYP4Z1 inhibitor. *European Journal of Medicinal Chemistry*, **2021**, 215, 113255	6.8	8
56	Design, synthesis, antibacterial activity evaluation and molecular modeling studies of new sulfonamides containing a sulfathiazole moiety. *New Journal of Chemistry*, **2021**, 45, 8166-8177	3.6	8
55	A common polymorphic variant of UGT1A5 displays increased activity due to optimized cofactor binding. *FEBS Letters*, **2018**, 592, 1837-1846	3.8	7
54	Identification and characterization of a novel chemotype for human TLR8 inhibitors. *European Journal of Medicinal Chemistry*, **2019**, 179, 744-752	6.8	7
53	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, 1002-9	3.4	7
52	Structural determinants of diphenethylamines for interaction with the □-opioid receptor: Synthesis, pharmacology and molecular modeling studies. *Bioorganic and Medicinal Chemistry Letters*, **2016**, 26, 4769-4774	2.9	7
51	Systematic Data Mining Reveals Synergistic H3R/MCHR1 Ligands. *ACS Medicinal Chemistry Letters*, **2017**, 8, 648-653	4.3	6
50	Pharmacophore Identification and Pseudo-Receptor Modeling **2015**, 489-510		6

49	HuskinDB, a database for skin permeation of xenobiotics. *Scientific Data*, **2020**, 7, 426	8.2	6
48	N-Phenethyl Substitution in 14-Methoxy-N-methylmorphinan-6-ones Turns Selective Opioid Receptor Ligands into Dual /Opioid Receptor Agonists. *Scientific Reports*, **2020**, 10, 5653	4.9	6
47	Discovery of Michael acceptor containing 1,4-dihydropyridines as first covalent inhibitors of L-/T-type calcium channels. *Bioorganic Chemistry*, **2019**, 91, 103187	5.1	6
46	ACE2-Variants Indicate Potential SARS-CoV-2-Susceptibility in Animals: An Extensive Molecular Dynamics Study		6
45	Structural insights into understudied human cytochrome P450 enzymes. *Drug Discovery Today*, **2021**, 26, 2456-2464	8.8	6
44	In Search for Multi-Target Ligands as Potential Agents for Diabetes Mellitus and Its Complications-A Structure-Activity Relationship Study on Inhibitors of Aldose Reductase and Protein Tyrosine Phosphatase 1B. *Molecules*, **2021**, 26,	4.8	6
43	Novel BQCA- and TBPB-Derived M Receptor Hybrid Ligands: Orthosteric Carbachol Differentially Regulates Partial Agonism. *ChemMedChem*, **2019**, 14, 1349-1358	3.7	5
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41	Design and synthesis of 3,5-substituted 1,2,4-oxadiazoles as catalytic inhibitors of human DNA topoisomerase II *Bioorganic Chemistry*, **2020**, 99, 103828	5.1	5
40	Discovery of Sanggenon G as a natural cell-permeable small-molecular weight inhibitor of X-linked inhibitor of apoptosis protein (XIAP). *FEBS Open Bio*, **2014**, 4, 659-71	2.7	5
39	Amylase Modulation: Discovery of Inhibitors Using a Multi-Pharmacophore Approach for Virtual Screening. *ChemMedChem*, **2016**, 11, 2372-2377	3.7	5
38	New Proluciferin Substrates for Human CYP4 Family Enzymes. *Applied Biochemistry and Biotechnology*, **2021**, 193, 218-237	3.2	5
37	Identification and validation of a novel dual small-molecule TLR2/8 antagonist. *Biochemical Pharmacology*, **2020**, 177, 113957	6	4
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35	Discovery of novel amylase inhibitors using structure-based drug design. *Journal of Cheminformatics*, **2014**, 6,	8.6	4
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