

Gerhard Wolber

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Validated Capillary Zone Electrophoresis Method for Impurity Profiling and Determination of Nill(3-OMe-Salophene). <i>Separations</i> , 2022 , 9, 25	3.1	1
191	Metabolism of the antipsychotic drug olanzapine by CYP3A43.. <i>Xenobiotica</i> , 2022 , 1-29	2	0
190	In Vitro, In Vivo and In Silico Characterization of a Novel Kappa-Opioid Receptor Antagonist. <i>Pharmaceuticals</i> , 2022 , 15, 680	5.2	1
189	Discovery of a novel potent cytochrome P450 CYP4Z1 inhibitor. <i>European Journal of Medicinal Chemistry</i> , 2021 , 215, 113255	6.8	8
188	Antinociceptive Efficacy of the μ -Opioid/Nociceptin Peptide-Based Hybrid KGNOP1 in Inflammatory Pain without Rewarding Effects in Mice: An Experimental Assessment and Molecular Docking. <i>Molecules</i> , 2021 , 26,	4.8	3
187	Chemische Evolution antiviraler Wirkstoffe gegen Enterovirus D68 durch Proteintemplat-gesteuerte Knoevenagelreaktionen. <i>Angewandte Chemie</i> , 2021 , 133, 13405-13413	3.6	0
186	Chemical Evolution of Antivirals Against Enterovirus D68 through Protein-Templated Knoevenagel Reactions. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 13294-13301	16.4	1
185	Corticosteroid Biosynthesis Revisited: No Direct Hydroxylation of Pregnenolone by Steroid 21-Hydroxylase. <i>Frontiers in Endocrinology</i> , 2021 , 12, 633785	5.7	0
184	Structural insights into understudied human cytochrome P450 enzymes. <i>Drug Discovery Today</i> , 2021 , 26, 2456-2464	8.8	6
183	New Proluciferin Substrates for Human CYP4 Family Enzymes. <i>Applied Biochemistry and Biotechnology</i> , 2021 , 193, 218-237	3.2	5
182	Design, synthesis, antibacterial activity evaluation and molecular modeling studies of new sulfonamides containing a sulfathiazole moiety. <i>New Journal of Chemistry</i> , 2021 , 45, 8166-8177	3.6	8
181	Exploiting Water Dynamics for Pharmacophore Screening. <i>Methods in Molecular Biology</i> , 2021 , 2266, 227-238	1.4	
180	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. <i>Molecules</i> , 2021 , 26,	4.8	6
179	ACE2-Variants Indicate Potential SARS-CoV-2-Susceptibility in Animals: A Molecular Dynamics Study. <i>Molecular Informatics</i> , 2021 , 40, e2100031	3.8	2
178	Further hit optimization of 6-(trifluoromethyl)pyrimidin-2-amine based TLR8 modulators: Synthesis, biological evaluation and structure-activity relationships. <i>European Journal of Medicinal Chemistry</i> , 2021 , 225, 113809	6.8	0
177	A convenient test system for the identification of CYP4V2 inhibitors. <i>Molecular Vision</i> , 2021 , 27, 601-607	2.3	
176	HuskinDB, a database for skin permeation of xenobiotics. <i>Scientific Data</i> , 2020 , 7, 426	8.2	6

175	Mechanistic Understanding of Peptide Analogues, DALDA, [Dmt]DALDA, and KGOP01, Binding to the mu Opioid Receptor. <i>Molecules</i> , 2020 , 25,	4.8	9
174	Catching a Moving Target: Comparative Modeling of Flaviviral NS2B-NS3 Reveals Small Molecule Zika Protease Inhibitors. <i>ACS Medicinal Chemistry Letters</i> , 2020 , 11, 514-520	4.3	8
173	Next generation 3D pharmacophore modeling. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020 , 10, e1468	7.9	49
172	Importance of asparagine-381 and arginine-487 for substrate recognition in CYP4Z1. <i>Biochemical Pharmacology</i> , 2020 , 174, 113850	6	12
171	Identification and validation of a novel dual small-molecule TLR2/8 antagonist. <i>Biochemical Pharmacology</i> , 2020 , 177, 113957	6	4
170	Design and synthesis of 3,5-substituted 1,2,4-oxadiazoles as catalytic inhibitors of human DNA topoisomerase II β . <i>Bioorganic Chemistry</i> , 2020 , 99, 103828	5.1	5
169	N-Phenethyl Substitution in 14-Methoxy-N-methylmorphinan-6-ones Turns Selective μ Opioid Receptor Ligands into Dual μ / κ Opioid Receptor Agonists. <i>Scientific Reports</i> , 2020 , 10, 5653	4.9	6
168	Biological Characterization, Mechanistic Investigation and Structure-Activity Relationships of Chemically Stable TLR2 Antagonists. <i>ChemMedChem</i> , 2020 , 15, 1364-1371	3.7	2
167	Corticosteroid Biosynthesis Revisited: Substrate Specificity of Steroid 21-Hydroxylase. <i>FASEB Journal</i> , 2020 , 34, 1-1	0.9	
166	The Role of Orthosteric Building Blocks of Bitopic Ligands for Muscarinic M1 Receptors. <i>ACS Omega</i> , 2020 , 5, 31706-31715	3.9	2
165	The novel small-molecule antagonist MMG-11 preferentially inhibits TLR2/1 signaling. <i>Biochemical Pharmacology</i> , 2020 , 171, 113687	6	11
164	Functional Expression of All Human Sulfotransferases in Fission Yeast, Assay Development, and Structural Models for Isoforms SULT4A1 and SULT6B1. <i>Biomolecules</i> , 2020 , 10,	5.9	4
163	A benzoxazole derivative as an inhibitor of anaerobic choline metabolism by human gut microbiota. <i>RSC Medicinal Chemistry</i> , 2020 , 11, 1402-1412	3.5	2
162	Ligand-Specific Allosteric Coupling Controls G-Protein-Coupled Receptor Signaling. <i>ACS Pharmacology and Translational Science</i> , 2020 , 3, 859-867	5.9	10
161	Biased Ligands Differentially Shape the Conformation of the Extracellular Loop Region in 5-HT Receptors. <i>International Journal of Molecular Sciences</i> , 2020 , 21,	6.3	4
160	PyRod Enables Rational Homology Model-based Virtual Screening Against MCHR1. <i>Molecular Informatics</i> , 2020 , 39, e2000020	3.8	1
159	Design and evaluation of non-carboxylate 5-arylidene-2-thioxo-4-imidazolidinones as novel non-competitive inhibitors of protein tyrosine phosphatase 1B. <i>Bioorganic Chemistry</i> , 2019 , 92, 103211	5.1	8
158	Mining large databases to find new leads with low similarity to known actives: application to find new DPP-IV inhibitors. <i>Future Medicinal Chemistry</i> , 2019 , 11, 1387-1401	4.1	1

157	Fine-mapping of the substrate specificity of human steroid 21-hydroxylase (CYP21A2). <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2019 , 194, 105446	5.1	10
156	PyRod: Tracing Water Molecules in Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 2818-2829	6.1	9
155	Functional characterization and mechanistic modeling of the human cytochrome P450 enzyme CYP4A22. <i>FEBS Letters</i> , 2019 , 593, 2214-2225	3.8	13
154	Ligand-guided homology modeling drives identification of novel histamine H3 receptor ligands. <i>PLoS ONE</i> , 2019 , 14, e0218820	3.7	12
153	Novel BQCA- and TBPB-Derived M Receptor Hybrid Ligands: Orthosteric Carbachol Differentially Regulates Partial Agonism. <i>ChemMedChem</i> , 2019 , 14, 1349-1358	3.7	5
152	N-methyl-D-aspartate receptor dysfunction by unmutated human antibodies against the NR1 subunit. <i>Annals of Neurology</i> , 2019 , 85, 771-776	9.4	29
151	Strategies for the discovery of biased GPCR ligands. <i>Drug Discovery Today</i> , 2019 , 24, 1031-1037	8.8	22
150	Fluorination of Photoswitchable Muscarinic Agonists Tunes Receptor Pharmacology and Photochromic Properties. <i>Journal of Medicinal Chemistry</i> , 2019 , 62, 3009-3020	8.3	14
149	Comparison of the three SARMS RAD-140, GLPG0492 and GSK-2881078 in two different in vitro bioassays, and in an in silico androgen receptor binding assay. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2019 , 189, 81-86	5.1	5
148	Assessment of Flexible Shape Complementarity: New Opportunities to Explain and Induce Selectivity in Ligands of Protein Tyrosine Phosphatase 1B. <i>Molecular Informatics</i> , 2019 , 38, e1800141	3.8	1
147	Discovery of Michael acceptor containing 1,4-dihydropyridines as first covalent inhibitors of L-/T-type calcium channels. <i>Bioorganic Chemistry</i> , 2019 , 91, 103187	5.1	6
146	Identification and characterization of a novel chemotype for human TLR8 inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2019 , 179, 744-752	6.8	7
145	Combined chemical and biotechnological production of 20DH-NorDHCMT, a long-term metabolite of Oral-Turinabol (DHCMT). <i>Journal of Inorganic Biochemistry</i> , 2018 , 183, 165-171	4.2	18
144	Pharmacophore Perception and Applications 2018 , 259-282		1
143	Identification of 2-thioxoimidazolidin-4-one derivatives as novel noncovalent proteasome and immunoproteasome inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2018 , 28, 278-283	2.9	4
142	Phenylthiomethyl Ketone-Based Fragments Show Selective and Irreversible Inhibition of Enteroviral 3C Proteases. <i>Journal of Medicinal Chemistry</i> , 2018 , 61, 1218-1230	8.3	14
141	A common polymorphic variant of UGT1A5 displays increased activity due to optimized cofactor binding. <i>FEBS Letters</i> , 2018 , 592, 1837-1846	3.8	7
140	Identification of a pyrogallol derivative as a potent and selective human TLR2 antagonist by structure-based virtual screening. <i>Biochemical Pharmacology</i> , 2018 , 154, 148-160	6	13

139	Androgen- and estrogen-receptor mediated activities of 4-hydroxytestosterone, 4-hydroxyandrostenedione and their human metabolites in yeast based assays. <i>Toxicology Letters</i> , 2018 , 292, 39-45	4.4	3
138	Nuclear transport of the human aryl hydrocarbon receptor and subsequent gene induction relies on its residue histidine 291. <i>Archives of Toxicology</i> , 2018 , 92, 1151-1160	5.8	4
137	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. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2018 , 28, 3712-3720	2.9	22
136	Binding mechanism investigations guiding the synthesis of novel condensed 1,4-dihydropyridine derivatives with L-/T-type calcium channel blocking activity. <i>European Journal of Medicinal Chemistry</i> , 2018 , 155, 1-12	6.8	23
135	Systematic Data Mining Reveals Synergistic H3R/MCHR1 Ligands. <i>ACS Medicinal Chemistry Letters</i> , 2017 , 8, 648-653	4.3	6
134	Ligand-Specific Restriction of Extracellular Conformational Dynamics Constrains Signaling of the M Muscarinic Receptor. <i>ACS Chemical Biology</i> , 2017 , 12, 1743-1748	4.9	18
133	Legacy data sharing to improve drug safety assessment: the eTOX project. <i>Nature Reviews Drug Discovery</i> , 2017 , 16, 811-812	64.1	37
132	Arginase Structure and Inhibition: Catalytic Site Plasticity Reveals New Modulation Possibilities. <i>Scientific Reports</i> , 2017 , 7, 13616	4.9	21
131	Efficient substrate screening and inhibitor testing of human CYP4Z1 using permeabilized recombinant fission yeast. <i>Biochemical Pharmacology</i> , 2017 , 146, 174-187	6	29
130	Synthesis, crystallographic characterization, molecular docking and biological activity of isoquinoline derivatives. <i>Chemistry Central Journal</i> , 2017 , 11, 103		8
129	Enhanced immunostimulatory activity of in silico discovered agonists of Toll-like receptor 2 (TLR2). <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2017 , 1861, 2680-2689	4	14
128	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. <i>European Journal of Medicinal Chemistry</i> , 2017 , 127, 840-858	6.8	23
127	Balancing Inflammation: Computational Design of Small-Molecule Toll-like Receptor Modulators. <i>Trends in Pharmacological Sciences</i> , 2017 , 38, 155-168	13.2	21
126	Anthocyanin composition, antioxidant efficiency, and α -amylase inhibitor activity of different Hungarian sour cherry varieties (<i>Prunus cerasus</i> L.). <i>Food Chemistry</i> , 2016 , 194, 222-9	8.5	69
125	Immunoproteasome-Selective Inhibitors: A Promising Strategy to Treat Hematologic Malignancies, Autoimmune and Inflammatory Diseases. <i>Current Medicinal Chemistry</i> , 2016 , 23, 1217-38	4.3	27
124	Molecular insight on the binding of NNRTI to K103N mutated HIV-1 RT: molecular dynamics simulations and dynamic pharmacophore analysis. <i>Molecular BioSystems</i> , 2016 , 12, 3385-3395		21
123	Ligand Binding Ensembles Determine Graded Agonist Efficacies at a G Protein-coupled Receptor. <i>Journal of Biological Chemistry</i> , 2016 , 291, 16375-89	5.4	50
122	More than a look into a crystal ball: protein structure elucidation guided by molecular dynamics simulations. <i>Drug Discovery Today</i> , 2016 , 21, 1799-1805	8.8	37

121	Irreversible inhibitors of the 3C protease of Coxsackie virus through templated assembly of protein-binding fragments. <i>Nature Communications</i> , 2016 , 7, 12761	17.4	22
120	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. <i>Journal of Cheminformatics</i> , 2016 , 8, 18	8.6	
119	Acute myeloid leukaemia-derived Langerhans-like cells enhance Th1 polarization upon TLR2 engagement. <i>Pharmacological Research</i> , 2016 , 105, 44-53	10.2	18
118	In Silico Prediction of Human Sulfotransferase 1E1 Activity Guided by Pharmacophores from Molecular Dynamics Simulations. <i>Journal of Biological Chemistry</i> , 2016 , 291, 58-71	5.4	21
117	In silico identification and in vitro activity of new pancreatic lipase inhibitors. <i>Planta Medica</i> , 2016 , 81, S1-S381	3.1	
116	Polyacetylenes and alkamides as modulators of PPAR γ activity and promising candidates for the treatment of type 2 diabetes. <i>Planta Medica</i> , 2016 , 81, S1-S381	3.1	
115	Chemoenzymatic Synthesis of Nonasulfated Tetrahyaluronan with a Paramagnetic Tag for Studying Its Complex with Interleukin-10. <i>Chemistry - A European Journal</i> , 2016 , 22, 5563-74	4.8	29
114	Identification of noncovalent proteasome inhibitors with high selectivity for chymotrypsin-like activity by a multistep structure-based virtual screening. <i>European Journal of Medicinal Chemistry</i> , 2016 , 121, 578-591	6.8	18
113	Structural determinants of diphenethylamines for interaction with the μ opioid receptor: Synthesis, pharmacology and molecular modeling studies. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2016 , 26, 4769-4774	2.9	7
112	New telmisartan-derived PPAR γ agonists: Impact of the 3D-binding mode on the pharmacological profile. <i>European Journal of Medicinal Chemistry</i> , 2016 , 124, 138-152	6.8	17
111	α -Amylase Modulation: Discovery of Inhibitors Using a Multi-Pharmacophore Approach for Virtual Screening. <i>ChemMedChem</i> , 2016 , 11, 2372-2377	3.7	5
110	The impact of molecular dynamics on drug design: applications for the characterization of ligand-macromolecule complexes. <i>Drug Discovery Today</i> , 2015 , 20, 686-702	8.8	135
109	3D-QSAR, design, synthesis and characterization of trisubstituted harmine derivatives with in vitro antiproliferative properties. <i>European Journal of Medicinal Chemistry</i> , 2015 , 94, 45-55	6.8	16
108	Structure versus function-The impact of computational methods on the discovery of specific GPCR-ligands. <i>Bioorganic and Medicinal Chemistry</i> , 2015 , 23, 3907-12	3.4	21
107	Pharmacophore Identification and Pseudo-Receptor Modeling 2015 , 489-510		6
106	Identification of PPAR γ Agonists from Natural Sources Using Different In Silico Approaches. <i>Planta Medica</i> , 2015 , 81, 488-94	3.1	15
105	Furan-based benzene mono- and dicarboxylic acid derivatives as multiple inhibitors of the bacterial Mur ligases (MurC-MurF): experimental and computational characterization. <i>Journal of Computer-Aided Molecular Design</i> , 2015 , 29, 541-60	4.2	18
104	Polyacetylenes from carrots (<i>Daucus carota</i>) improve glucose uptake in vitro in adipocytes and myotubes. <i>Food and Function</i> , 2015 , 6, 2135-44	6.1	24

103	Selective inhibitors of the protein tyrosine phosphatase SHP2 block cellular motility and growth of cancer cells in vitro and in vivo. <i>ChemMedChem</i> , 2015 , 10, 815-26	3.7	51
102	From carbohydrates to drug-like fragments: Rational development of novel α -amylase inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2015 , 23, 6725-32	3.4	16
101	Computational close up on protein-protein interactions: how to unravel the invisible using molecular dynamics simulations?. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2015 , 5, 345-359	7.9	27
100	Structural Characteristics of the Allosteric Binding Site Represent a Key to Subtype Selective Modulators of Muscarinic Acetylcholine Receptors. <i>Molecular Informatics</i> , 2015 , 34, 526-30	3.8	19
99	Coiled-coils in phage display screening: insight into exceptional selectivity provided by molecular dynamics. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 495-500	6.1	2
98	Ecdysteroids: A novel class of anabolic agents?. <i>Biology of Sport</i> , 2015 , 32, 169-73	4.3	45
97	Peptide-based proteasome inhibitors in anticancer drug design. <i>Medicinal Research Reviews</i> , 2014 , 34, 1001-69	14.4	40
96	Synthesis, biological evaluation, and docking studies of new 2-furylbenzimidazoles as anti-angiogenic agents: part II. <i>Archiv Der Pharmazie</i> , 2014 , 347, 291-304	4.3	13
95	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. <i>European Journal of Medicinal Chemistry</i> , 2014 , 71, 112-27	6.8	40
94	Impact of fluorination on proteolytic stability of peptides: a case study with α -chymotrypsin and pepsin. <i>Amino Acids</i> , 2014 , 46, 2733-44	3.5	28
93	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. <i>European Journal of Medicinal Chemistry</i> , 2014 , 86, 122-32	6.8	78
92	Inhibitor design strategy based on an enzyme structural flexibility: a case of bacterial MurD ligase. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 1451-66	6.1	17
91	Inhibitory potency of flavonoid derivatives on influenza virus neuraminidase. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2014 , 24, 4312-7	2.9	34
90	Optimization of peptidomimetic boronates bearing a P3 bicyclic scaffold as proteasome inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2014 , 83, 1-14	6.8	22
89	Selected cytotoxic gold compounds cause significant inhibition of 20S proteasome catalytic activities. <i>Journal of Inorganic Biochemistry</i> , 2014 , 141, 79-82	4.2	22
88	Development of novel selective peptidomimetics containing a boronic acid moiety, targeting the 20S proteasome as anticancer agents. <i>ChemMedChem</i> , 2014 , 9, 1801-16	3.7	13
87	Discovery of Sanggenon G as a natural cell-permeable small-molecular weight inhibitor of X-linked inhibitor of apoptosis protein (XIAP). <i>FEBS Open Bio</i> , 2014 , 4, 659-71	2.7	5
86	Prospective virtual screening in a sparse data scenario: design of small-molecule TLR2 antagonists. <i>ChemMedChem</i> , 2014 , 9, 813-22	3.7	27

85	Combining pharmacophore- and MD-based modelling for phase II metabolism prediction. <i>Journal of Cheminformatics</i> , 2014 , 6, O15	8.6	
84	Balancing selectivity vs stability using molecular dynamics and umbrella sampling. <i>Journal of Cheminformatics</i> , 2014 , 6, O22	8.6	
83	Using structure- and Ligand-based pharmacophores as filters to discriminate Human Aryl Sulfotransferase 1A1 (SUL1A1) binders into substrates and inhibitors. <i>Journal of Cheminformatics</i> , 2014 , 6,	8.6	78
82	Discovery of novel α -amylase inhibitors using structure-based drug design. <i>Journal of Cheminformatics</i> , 2014 , 6,	8.6	4
81	An unusual interstrand H-bond stabilizes the heteroassembly of helical α -himeras with natural peptides. <i>ACS Chemical Biology</i> , 2014 , 9, 613-6	4.9	9
80	Dualsteric muscarinic antagonists--orthosteric binding pose controls allosteric subtype selectivity. <i>Journal of Medicinal Chemistry</i> , 2014 , 57, 6739-50	8.3	25
79	Identification of a new series of amides as non-covalent proteasome inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2014 , 76, 1-9	6.8	20
78	Benzene-1,3-dicarboxylic acid 2,5-dimethylpyrrole derivatives as multiple inhibitors of bacterial Mur ligases (MurC-MurF). <i>Bioorganic and Medicinal Chemistry</i> , 2014 , 22, 4124-34	3.4	27
77	Isomeric C12-alkamides from the roots of <i>Echinacea purpurea</i> improve basal and insulin-dependent glucose uptake in 3T3-L1 adipocytes. <i>Planta Medica</i> , 2014 , 80, 1712-20	3.1	9
76	α - and β -Amino Acids at α -Helical Interfaces: Toward the Formation of Highly Stable Foldameric Coiled Coils. <i>ACS Medicinal Chemistry Letters</i> , 2014 , 5, 1300-3	4.3	8
75	Design, synthesis and structure-activity relationship of novel quinoxaline derivatives as cancer chemopreventive agent by inhibition of tyrosine kinase receptor. <i>European Journal of Medicinal Chemistry</i> , 2013 , 69, 115-24	6.8	32
74	Isolation of a novel thioflavin S-derived compound that inhibits BAG-1-mediated protein interactions and targets BRAF inhibitor-resistant cell lines. <i>Molecular Cancer Therapeutics</i> , 2013 , 12, 2400-14	6.1	18
73	Butyltin(IV) benzoates: inhibition of thioredoxin reductase, tumor cell growth inhibition, and interactions with proteins. <i>ChemMedChem</i> , 2013 , 8, 256-64	3.7	23
72	Design, synthesis, inhibition studies, and molecular modeling of pepstatin analogues addressing different secreted aspartic proteinases of <i>Candida albicans</i> . <i>Biochemical Pharmacology</i> , 2013 , 85, 881-7	6	14
71	The μ opioid receptor and ligands acting at the μ opioid receptor, as therapeutics and potential therapeutics. <i>Current Pharmaceutical Design</i> , 2013 , 19, 7415-34	3.3	44
70	Development of peptidomimetic boronates as proteasome inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2013 , 64, 23-34	6.8	31
69	Molecular dynamics simulation and linear interaction energy study of D-Glu-based inhibitors of the MurD ligase. <i>Journal of Computer-Aided Molecular Design</i> , 2013 , 27, 723-38	4.2	23
68	Interruption of the ionic lock in the bradykinin B2 receptor results in constitutive internalization and turns several antagonists into strong agonists. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2013 , 344, 85-95	4.7	13

67	NSC23766, a widely used inhibitor of Rac1 activation, additionally acts as a competitive antagonist at muscarinic acetylcholine receptors. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2013 , 347, 69-79	4.7	54
66	Current μ -opioid receptor ligands and discovery of a new molecular scaffold as a μ -opioid receptor antagonist using pharmacophore-based virtual screening. <i>Current Pharmaceutical Design</i> , 2013 , 19, 7362-72	3.7	12
65	Synthesis and biological assessment of novel 2-thiazolylhydrazones and computational analysis of their recognition by monoamine oxidase B. <i>European Journal of Medicinal Chemistry</i> , 2012 , 48, 284-95	6.8	29
64	Identification of HIV-1 reverse transcriptase dual inhibitors by a combined shape-, 2D-fingerprint- and pharmacophore-based virtual screening approach. <i>European Journal of Medicinal Chemistry</i> , 2012 , 50, 216-29	6.8	55
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. <i>European Journal of Medicinal Chemistry</i> , 2012 , 50, 332-43	6.8	29
62	Pharmacophore-based discovery of a novel cytosolic phospholipase A(2)-inhibitor. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012 , 22, 1202-7	2.9	9
61	Binding characteristics of [3H]-JSM10292: a new cell membrane-permeant non-peptide bradykinin B2 receptor antagonist. <i>British Journal of Pharmacology</i> , 2012 , 167, 839-53	8.6	9
60	Influence of chlorine or fluorine substitution on the estrogenic properties of 1-alkyl-2,3,5-tris(4-hydroxyphenyl)-1H-pyrroles. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 9607-18	8.3	17
59	Novel pharmacological chaperones that correct phenylketonuria in mice. <i>Human Molecular Genetics</i> , 2012 , 21, 1877-87	5.6	50
58	In silico virtual screening approaches for anti-viral drug discovery. <i>Drug Discovery Today: Technologies</i> , 2012 , 9, e219-25	7.1	44
57	Identification of PPARgamma partial agonists of natural origin (I): development of a virtual screening procedure and in vitro validation. <i>PLoS ONE</i> , 2012 , 7, e50816	3.7	38
56	Identification of novel liver X receptor activators by structure-based modeling. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 1391-400	6.1	13
55	Computational tools for in silico fragment-based drug design. <i>Current Topics in Medicinal Chemistry</i> , 2012 , 12, 1935-43	3	20
54	Pharmacophore modeling and virtual screening for novel acidic inhibitors of microsomal prostaglandin G synthase-1 (mPGES-1). <i>Journal of Medicinal Chemistry</i> , 2011 , 54, 3163-74	8.3	48
53	Characterization of activity and binding mode of glycyrrhetic acid derivatives inhibiting 11 β -hydroxysteroid dehydrogenase type 2. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2011 , 125, 129-42	5.1	52
52	Identification of chemically diverse, novel inhibitors of 17 β -hydroxysteroid dehydrogenase type 3 and 5 by pharmacophore-based virtual screening. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2011 , 125, 148-61	5.1	30
51	Computational Approaches for the Discovery of Natural Lead Structures 2011 , 97-132		
50	Predicting cyclooxygenase inhibition by three-dimensional pharmacophoric profiling. Part II: Identification of enzyme inhibitors from Prasapalai, a Thai traditional medicine. <i>Phytomedicine</i> , 2011 , 18, 119-33	6.5	13

49	Pharmacophore-based discovery of FXR-agonists. Part II: identification of bioactive triterpenes from <i>Ganoderma lucidum</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2011 , 19, 6779-91	3-4	48
48	Pharmacophore-based discovery of FXR agonists. Part I: Model development and experimental validation. <i>Bioorganic and Medicinal Chemistry</i> , 2011 , 19, 7168-80	3-4	43
47	Development of novel peptidomimetics containing a vinyl sulfone moiety as proteasome inhibitors. <i>ChemMedChem</i> , 2011 , 6, 1228-37	3-7	38
46	Development of 2,3,5-triaryl-1H-pyrroles as estrogen receptor selective ligands. <i>ChemMedChem</i> , 2011 , 6, 2055-62	3-7	4
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