Xiaomin Luo

List of Publications by Year in descending order

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131	7,261	71102	62596
papers	citations	41 h-index	80 g-index

136	136	136	8972
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Predicting protein-protein interactions based only on sequences information. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 4337-4341.	7.1	826
2	Halogen Bondingâ€"A Novel Interaction for Rational Drug Design?. Journal of Medicinal Chemistry, 2009, 52, 2854-2862.	6.4	524
3	Pushing the Boundaries of Molecular Representation for Drug Discovery with the Graph Attention Mechanism. Journal of Medicinal Chemistry, 2020, 63, 8749-8760.	6.4	402
4	TarFisDock: a web server for identifying drug targets with docking approach. Nucleic Acids Research, 2006, 34, W219-W224.	14.5	372
5	In silicoADME/T modelling for rational drug design. Quarterly Reviews of Biophysics, 2015, 48, 488-515.	5.7	250
6	PDTD: a web-accessible protein database for drug target identification. BMC Bioinformatics, 2008, 9, 104.	2.6	249
7	Conformational transition of amyloid Î²-peptide. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 5403-5407.	7.1	238
8	TransformerCPI: improving compoundâ€"protein interaction prediction by sequence-based deep learning with self-attention mechanism and label reversal experiments. Bioinformatics, 2020, 36, 4406-4414.	4.1	190
9	Cinanserin Is an Inhibitor of the 3C-Like Proteinase of Severe Acute Respiratory Syndrome Coronavirus and Strongly Reduces Virus Replication In Vitro. Journal of Virology, 2005, 79, 7095-7103.	3.4	185
10	Virtual Screening on Natural Products for Discovering Active Compounds and Target Information. Current Medicinal Chemistry, 2003, 10, 2327-2342.	2.4	123
11	Paeoniflorin attenuates neuroinflammation and dopaminergic neurodegeneration in the MPTP model of Parkinson's disease by activation of adenosine A1 receptor. British Journal of Pharmacology, 2006, 148, 314-325.	5.4	114
12	Progress in Clinical, Pharmacological, Chemical and Structural Biological Studies of Huperzine A: A Drug of Traditional Chinese Medicine Origin for the Treatment of Alzheimers Disease. Current Medicinal Chemistry, 2003, 10, 2231-2252.	2.4	105
13	Nucleocapsid protein of SARS coronavirus tightly binds to human cyclophilin A. Biochemical and Biophysical Research Communications, 2004, 321, 557-565.	2.1	104
14	How Does Huperzine A Enter and Leave the Binding Gorge of Acetylcholinesterase? Steered Molecular Dynamics Simulations. Journal of the American Chemical Society, 2003, 125, 11340-11349.	13.7	94
15	Câ^'XÂ·Â·Â·H Contacts in Biomolecular Systems: How They Contribute to Proteinâ^'Ligand Binding Affinity. Journal of Physical Chemistry B, 2009, 113, 12615-12621.	2.6	88
16	Pharmacophore-based virtual screening versus docking-based virtual screening: a benchmark comparison against eight targets. Acta Pharmacologica Sinica, 2009, 30, 1694-1708.	6.1	86
17	Steered Molecular Dynamics Simulation on the Binding of NNRTI to HIV-1 RT. Biophysical Journal, 2003, 84, 3547-3563.	0.5	77
18	3D-QSAR Model of Flavonoids Binding at Benzodiazepine Site in GABAA Receptors. Journal of Medicinal Chemistry, 2001, 44, 1883-1891.	6.4	75

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19	Site of metabolism prediction for six biotransformations mediated by cytochromes P450. Bioinformatics, 2009, 25, 1251-1258.	4.1	72
20	Focused Combinatorial Library Design Based on Structural Diversity, Druglikeness and Binding Affinity Score. ACS Combinatorial Science, 2005, 7, 398-406.	3.3	69
21	Molecular Dynamics Simulations on SDF-1Î±: Binding with CXCR4 Receptor. Biophysical Journal, 2003, 84, 171-184.	0.5	67
22	A New Rapid and Effective Chemistry Space Filter in Recognizing a Druglike Database. Journal of Chemical Information and Modeling, 2005, 45, 856-862.	5.4	67
23	Molecular docking and 3-D-QSAR studies on the possible antimalarial mechanism of artemisinin analogues. Bioorganic and Medicinal Chemistry, 2002, 10, 2883-2891.	3.0	64
24	Conformational Dynamics of the Nicotinic Acetylcholine Receptor Channel:â€‰ A 35-ns Molecular Dynamics Simulation Study. Journal of the American Chemical Society, 2005, 127, 1291-1299.	13.7	64
25	Inhibitory Mode of 1,5-Diarylpyrazole Derivatives against Cyclooxygenase-2 and Cyclooxygenase-1:Â Molecular Docking and 3D QSAR Analyses. Journal of Medicinal Chemistry, 2002, 45, 4816-4827.	6.4	61
26	Computational Screening for Active Compounds Targeting Protein Sequences: Methodology and Experimental Validation. Journal of Chemical Information and Modeling, 2011, 51, 2821-2828.	5.4	61
27	Novel thiophene derivatives as PTP1B inhibitors with selectivity and cellular activity. Bioorganic and Medicinal Chemistry, 2010, 18, 1773-1782.	3.0	59
28	GAsDock: a new approach for rapid flexible docking based on an improved multi-population genetic algorithm. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 4671-4676.	2.2	56
29	Computational Simulations of Interactions of Scorpion Toxins with the Voltage-Gated Potassium Ion Channel. Biophysical Journal, 2004, 86, 3542-3555.	0.5	55
30	Possible Pathway(s) of Metyrapone Egress from the Active Site of Cytochrome P450 3A4: A Molecular Dynamics Simulation. Drug Metabolism and Disposition, 2007, 35, 689-696.	3.3	54
31	Dynamic Mechanism of E2020 Binding to Acetylcholinesterase:â€‰ A Steered Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2005, 109, 23730-23738.	2.6	53
32	Novel Bayesian classification models for predicting compounds blocking hERG potassium channels. Acta Pharmacologica Sinica, 2014, 35, 1093-1102.	6.1	53
33	TarPred: a web application for predicting therapeutic and side effect targets of chemical compounds. Bioinformatics, 2015, 31, 2049-2051.	4.1	52
34	Structure-Based Discovery of Potassium Channel Blockers from Natural Products. Chemistry and Biology, 2003, 10, 1103-1113.	6.0	50
35	POSSIBLE PATHWAY(S) OF TESTOSTERONE EGRESS FROM THE ACTIVE SITE OF CYTOCHROME P450 2B1: A STEERED MOLECULAR DYNAMICS SIMULATION. Drug Metabolism and Disposition, 2005, 33, 910-919.	3.3	50
36	Brownian Dynamics Simulations of the Recognition of the Scorpion Toxin Maurotoxin with the Voltage-Gated Potassium Ion Channels. Biophysical Journal, 2002, 83, 2370-2385.	0.5	49

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37	Molecular docking and 3D QSAR studies on 1-amino-2-phenyl-4-(piperidin-1-yl)-butanes based on the structural modeling of human CCR5 receptor. Bioorganic and Medicinal Chemistry, 2004, 12, 6193-6208.	3.0	48
38	In Silicotarget fishing: addressing a â€œBig Dataâ€•problem by ligand-based similarity rankings with data fusion. Journal of Cheminformatics, 2014, 6, 33.	6.1	48
39	Design, Synthesis, and Interaction Study of Quinazoline-2(1H)-thione Derivatives as Novel Potential Bcl-xL Inhibitors. Journal of Medicinal Chemistry, 2010, 53, 3465-3479.	6.4	47
40	Synthesis, characterization, in vitro antioxidant and hypoglycemic activities of selenium nanoparticles decorated with polysaccharides of Gracilaria lemaneiformis. International Journal of Biological Macromolecules, 2021, 193, 923-932.	7.5	47
41	Influence of the Water Molecule on Cationâ^Ï€ Interaction:Â Ab Initio Second Order MÃllerâ^Plesset Perturbation Theory (MP2) Calculations. Journal of Physical Chemistry B, 2005, 109, 5945-5949.	2.6	46
42	Brownian Dynamics Simulations of the Recognition of the Scorpion Toxin P05 with the Small-conductance Calcium-activated Potassium Channels. Journal of Molecular Biology, 2002, 318, 417-428.	4.2	45
43	Elucidating the Inhibiting Mode of AHPBA Derivatives against HIV-1 Protease and Building Predictive 3D-QSAR Models. Journal of Medicinal Chemistry, 2002, 45, 333-343.	6.4	43
44	Brownian Dynamics Simulations of Interaction Between Scorpion Toxin Lq2 and Potassium Ion Channel. Biophysical Journal, 2001, 80, 1659-1669.	0.5	42
45	Strategy for Discovering Chemical Inhibitors of Human Cyclophilin A:Â Focused Library Design, Virtual Screening, Chemical Synthesis and Bioassay. ACS Combinatorial Science, 2006, 8, 326-337.	3.3	42
46	An Improved PMF Scoring Function for Universally Predicting the Interactions of a Ligand with Protein, DNA, and RNA. Journal of Chemical Information and Modeling, 2008, 48, 1438-1447.	5.4	42
47	Synthesis and antitumor evaluation of novel 5-substituted-4-hydroxy-8-nitroquinazolines as EGFR signaling-targeted inhibitors. Bioorganic and Medicinal Chemistry, 2005, 13, 5613-5622.	3.0	40
48	Dopamine D1 Receptor Agonist and D2 Receptor Antagonist Effects of the Natural Product (â^')â€“Stepholidine: Molecular Modeling and Dynamics Simulations. Biophysical Journal, 2007, 93, 1431-1441.	0.5	38
49	Computational chemical biology and drug design: Facilitating protein structure, function, and modulation studies. Medicinal Research Reviews, 2018, 38, 914-950.	10.5	38
50	Machine-Learning-Guided Cocrystal Prediction Based on Large Data Base. Crystal Growth and Design, 2020, 20, 6610-6621.	3.0	38
51	Mechanism of the All-Î± to All-Î² Conformational Transition of RfaH-CTD: Molecular Dynamics Simulation and Markov State Model. Journal of Chemical Theory and Computation, 2014, 10, 2255-2264.	5.3	37
52	Thermodynamic and Structural Characterization of Halogen Bonding in Proteinâ€“Ligand Interactions: A Case Study of PDE5 and Its Inhibitors. Journal of Medicinal Chemistry, 2014, 57, 3588-3593.	6.4	37
53	Dynamic Mechanism for the Autophosphorylation of CheA Histidine Kinase:Â Molecular Dynamics Simulations. Journal of the American Chemical Society, 2005, 127, 11709-11719.	13.7	35
54	Aldehyde Oxidase Mediated Metabolism in Drug-like Molecules: A Combined Computational and Experimental Study. Journal of Medicinal Chemistry, 2017, 60, 2973-2982.	6.4	34

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55	QSAR analyses on ginkgolides and their analogues using CoMFA, CoMSIA, and HQSAR. Bioorganic and Medicinal Chemistry, 2005, 13, 313-322.	3.0	33
56	Non-Covalent Interactions with Aromatic Rings: Current Understanding and Implications for Rational Drug Design. Current Pharmaceutical Design, 2013, 19, 6522-6533.	1.9	33
57	Binding Investigation of Human 5-Lipoxygenase with Its Inhibitors by SPR Technology Correlating with Molecular Docking Simulation. Journal of Biochemistry, 2006, 139, 715-723.	1.7	32
58	Using support vector regression coupled with the genetic algorithm for predicting acute toxicity to the fathead minnow. SAR and QSAR in Environmental Research, 2010, 21, 559-570.	2.2	32
59	Discovering Potassium Channel Blockers from Synthetic Compound Database by Using Structure-Based Virtual Screening in Conjunction with Electrophysiological Assay. Journal of Medicinal Chemistry, 2007, 50, 83-93.	6.4	31
60	Knowledge-Based Scoring Functions in Drug Design: 2. Can the Knowledge Base Be Enriched?. Journal of Chemical Information and Modeling, 2011, 51, 386-397.	5.4	31
61	N-Methylformamideâ^'Benzene Complex as a Prototypical Peptide Nâ^'HÂ·Â·Â·Ï€ Hydrogen-Bonded System:Â Density Functional Theory and MP2 Studies. Journal of Organic Chemistry, 2003, 68, 7490-7495.	3.2	30
62	Estimation of acute oral toxicity in rat using local lazy learning. Journal of Cheminformatics, 2014, 6, 26.	6.1	30
63	Molecular docking and 3D-QSAR studies on the binding mechanism of statine-based peptidomimetics with Î²-secretase. Bioorganic and Medicinal Chemistry, 2005, 13, 2121-2131.	3.0	29
64	Indole derivatives as potent inhibitors of 5-lipoxygenase: Design, synthesis, biological evaluation, and molecular modeling. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 2414-2420.	2.2	29
65	Identification of novel thiadiazoloacrylamide analogues as inhibitors of dengue-2 virus NS2B/NS3 protease. Bioorganic and Medicinal Chemistry, 2014, 22, 6344-6352.	3.0	29
66	In silico site of metabolism prediction for human UGT-catalyzed reactions. Bioinformatics, 2014, 30, 398-405.	4.1	29
67	Mutagenic probability estimation of chemical compounds by a novel molecular electrophilicity vector and support vector machine. Bioinformatics, 2006, 22, 2099-2106.	4.1	28
68	Policresulen, a novel NS2B/NS3 protease inhibitor, effectively inhibits the replication of DENV2 virus in BHK-21 cells. Acta Pharmacologica Sinica, 2015, 36, 1126-1136.	6.1	28
69	A Density-Functional Study of the Mechanism for the Diastereoselective Epoxidation of Chiral Allylic Alcohols by the Titanium Peroxy Complexes. Journal of Organic Chemistry, 2002, 67, 1427-1435.	3.2	27
70	Estimation of elimination half-lives of organic chemicals in humans using gradient boosting machine. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 2664-2671.	2.4	27
71	Design, synthesis and antitumor evaluation of a new series of N-substituted-thiourea derivatives. Acta Pharmacologica Sinica, 2006, 27, 1259-1271.	6.1	26
72	A novel sulfonamide agent, MPSP-001, exhibits potent activity against human cancer cells in vitro through disruption of microtubule. Acta Pharmacologica Sinica, 2012, 33, 261-270.	6.1	26

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73	Identification and biochemical characterization of DC07090 as a novel potent small molecule inhibitor against human enterovirus 71 3C protease by structure-based virtual screening. European Journal of Medicinal Chemistry, 2016, 124, 981-991.	5.5	25
74	Drug repurposing against breast cancer by integrating drug-exposure expression profiles and drugâ€“drug links based on graph neural network. Bioinformatics, 2021, 37, 2930-2937.	4.1	25
75	Research progress in cation-Ï€ interactions. Science in China Series B: Chemistry, 2008, 51, 709-717.	0.8	24
76	Molecular Docking and 3D-QSAR Studies on Gag Peptide Analogue Inhibitors Interacting with Human Cyclophilin A. Journal of Medicinal Chemistry, 2002, 45, 5249-5259.	6.4	23
77	Molecular dynamics simulations of interaction between protein-tyrosine phosphatase 1B and a bidentate inhibitor1. Acta Pharmacologica Sinica, 2006, 27, 100-110.	6.1	23
78	Essential structural profile of a dual functional inhibitor against cyclooxygenase-2 (COX-2) and 5-lipoxygenase (5-LOX): Molecular docking and 3D-QSAR analyses on DHDMBF analogues. Bioorganic and Medicinal Chemistry, 2006, 14, 3428-3437.	3.0	23
79	Discovering novel 3-nitroquinolines as a new class of anticancer agents. Acta Pharmacologica Sinica, 2008, 29, 1529-1538.	6.1	23
80	Newp-Methylsulfonamido Phenylethylamine Analogues as Class III Antiarrhythmic Agents:Â Design, Synthesis, Biological Assay, and 3D-QSAR Analysis. Journal of Medicinal Chemistry, 2002, 45, 2953-2969.	6.4	22
81	Inhibitory mode of indole-2-carboxamide derivatives against HLGPa: molecular docking and 3D-QSAR analysesâ˜†. Bioorganic and Medicinal Chemistry, 2004, 12, 4147-4157.	3.0	22
82	Discovery of novel dual-action antidiabetic agents that inhibit glycogen phosphorylase and activate glucokinase. European Journal of Medicinal Chemistry, 2012, 58, 624-639.	5.5	22
83	Discovery of Novel Inhibitors Targeting the Menin-Mixed Lineage Leukemia Interface Using Pharmacophore- and Docking-Based Virtual Screening. Journal of Chemical Information and Modeling, 2016, 56, 1847-1855.	5.4	22
84	Computational analysis of molecular basis of 1:1 interactions of NRG-1Î² wild-type and variants with ErbB3 and ErbB4. Proteins: Structure, Function and Bioinformatics, 2005, 59, 742-756.	2.6	21
85	QSAR analyses on avian influenza virus neuraminidase inhibitors using CoMFA, CoMSIA, and HQSAR. Journal of Computer-Aided Molecular Design, 2006, 20, 549-566.	2.9	21
86	Understanding the regulation mechanisms of PAF receptor by agonists and antagonists: Molecular modeling and molecular dynamics simulation studies. Proteins: Structure, Function and Bioinformatics, 2007, 67, 41-52.	2.6	21
87	Conformational Transition and Energy Landscape of ErbB4 Activated by Neuregulin1Î²: One Microsecond Molecular Dynamics Simulations. Journal of the American Chemical Society, 2012, 134, 6720-6731.	13.7	21
88	Combinatorial Pharmacophore Modeling of Organic Cation Transporter 2 (OCT2) Inhibitors: Insights into Multiple Inhibitory Mechanisms. Molecular Pharmaceutics, 2013, 10, 4611-4619.	4.6	21
89	Identification of 15d-PGJ2 as an antagonist of farnesoid X receptor: Molecular modeling with biological evaluation. Steroids, 2013, 78, 813-822.	1.8	20
90	Molecular Insight into the Interaction between IFABP and PA by Using MMâ˜’PBSA and Alanine Scanning Methods. Journal of Physical Chemistry B, 2007, 111, 9104-9113.	2.6	19

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91	Molecular Dynamics Simulations on the Mechanism of Transporting Methylamine and Ammonia by Ammonium Transporter AmtB. Journal of Physical Chemistry B, 2010, 114, 15172-15179.	2.6	19
92	Blocking of the Nicotinic Acetylcholine Receptor Ion Channel by Chlorpromazine, a Noncompetitive Inhibitor:Â A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2006, 110, 20640-20648.	2.6	18
93	3D-QSAR study of 20 (S)-camptothecin analogs. Acta Pharmacologica Sinica, 2007, 28, 307-314.	6.1	18
94	A hybrid framework for improving uncertainty quantification in deep learning-based QSAR regression modeling. Journal of Cheminformatics, 2021, 13, 69.	6.1	18
95	Knowledge-Based Scoring Functions in Drug Design: 3. A Two-Dimensional Knowledge-Based Hydrogen-Bonding Potential for the Prediction of Proteinâ€“Ligand Interactions. Journal of Chemical Information and Modeling, 2011, 51, 2994-3004.	5.4	17
96	Elucidating inhibitory models of the inhibitors of epidermal growth factor receptor by docking and 3D-QSAR. Bioorganic and Medicinal Chemistry, 2004, 12, 2409-2417.	3.0	16
97	Efficient Synthesis of Î±-Aryl-/Heteroaryl-Substituted Î²-Amino Acids via Ni(II) Complex through the Suzuki Coupling Reaction. Journal of Organic Chemistry, 2009, 74, 5656-5659.	3.2	15
98	Estimation of Carcinogenicity Using Molecular Fragments Tree. Journal of Chemical Information and Modeling, 2012, 52, 1994-2003.	5.4	15
99	Combinatorial Pharmacophore Modeling of Multidrug and Toxin Extrusion Transporter 1 Inhibitors: a Theoretical Perspective for Understanding Multiple Inhibitory Mechanisms. Scientific Reports, 2015, 5, 13684.	3.3	15
100	Towards discovering dual functional inhibitors against both wild type and K103N mutant HIV-1 reverse transcriptases: molecular docking and QSAR studies on 4,1-benzoxazepinone analogues. Journal of Computer-Aided Molecular Design, 2006, 20, 281-293.	2.9	14
101	Tryptophan-containing dipeptide derivatives as potent PPARÎ³ antagonists: Design, synthesis, biological evaluation, and molecular modeling. European Journal of Medicinal Chemistry, 2008, 43, 2699-2716.	5.5	14
102	Machine Learning-Based Modeling of Drug Toxicity. Methods in Molecular Biology, 2018, 1754, 247-264.	0.9	14
103	Simulating the Interactions of Toxins with K+ Channels. Current Pharmaceutical Design, 2004, 10, 1057-1067.	1.9	14
104	Steered Molecular Dynamics Simulations on the â€œTail Helix Latchâ€•Hypothesis in the Gelsolin Activation Process. Biophysical Journal, 2002, 83, 753-762.	0.5	12
105	Expression and purification of the catalytic domain of human vascular endothelial growth factor receptor 2 for inhibitor screening. Biochimica Et Biophysica Acta - General Subjects, 2005, 1722, 254-261.	2.4	12
106	Pharmacophore-directed Homology Modeling and Molecular Dynamics Simulation of G Protein-coupled Receptor: Study of Possible Binding Modes of 5-HT2CReceptor Agonists. Acta Biochimica Et Biophysica Sinica, 2007, 39, 413-422.	2.0	12
107	Interaction Models of a Series of Oxadiazole-Substituted α-Isopropoxy Phenylpropanoic Acids Against PPARα and PPARγ: Molecular Modeling and Comparative Molecular Similarity Indices Analysis Studies. Protein and Peptide Letters, 2009, 16, 150-162.	0.9	12
108	Identification of Novel Small Molecules as Inhibitors of Hepatitis C Virus by Structure-Based Virtual Screening. International Journal of Molecular Sciences, 2013, 14, 22845-22856.	4.1	12

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109	Active Learning for Drug Design: A Case Study on the Plasma Exposure of Orally Administered Drugs. Journal of Medicinal Chemistry, 2021, 64, 16838-16853.	6.4	12
110	Molecular Dynamics of Nicotinic Acetylcholine Receptor Correlating Biological Functions. Current Protein and Peptide Science, 2006, 7, 195-200.	1.4	11
111	Hepatoprotective Effect and Potential Mechanism of Aqueous Extract from Phyllanthus emblica on Carbon-Tetrachloride-Induced Liver Fibrosis in Rats. Evidence-based Complementary and Alternative Medicine, 2021, 2021, 1-12.	1.2	11
112	Dynamic Mechanism of Fatty Acid Transport across Cellular Membranes through FadL: Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 13070-13078.	2.6	10
113	Fragment-based prediction of skin sensitization using recursive partitioning. Journal of Computer-Aided Molecular Design, 2011, 25, 885-893.	2.9	10
114	Deep Neural Network Classifier for Virtual Screening Inhibitors of (S)-Adenosyl-L-Methionine (SAM)-Dependent Methyltransferase Family. Frontiers in Chemistry, 2019, 7, 324.	3.6	10
115	Revisiting Aldehyde Oxidase Mediated Metabolism in Drug-like Molecules: An Improved Computational Model. Journal of Medicinal Chemistry, 2020, 63, 6523-6537.	6.4	10
116	Binding sensitivity of adefovir to the polymerase from different genotypes of HBV: molecular modeling, docking and dynamics simulation studies. Acta Pharmacologica Sinica, 2013, 34, 319-328.	6.1	9
117	Diterpenoids from the Root Bark of Pinus massoniana and Evaluation of Their Phosphodiesterase Type 4D Inhibitory Activity. Journal of Natural Products, 2020, 83, 1229-1237.	3.0	9
118	Discovery of Cyclic Peptidomimetic Ligands Targeting the Extracellular Domain of EGFR. Journal of Medicinal Chemistry, 2021, 64, 11219-11228.	6.4	9
119	Computational Models for Predicting Interactions with Membrane Transporters. Current Medicinal Chemistry, 2013, 20, 2118-2136.	2.4	8
120	Small molecule targeting CELF1 RNA-binding activity to control HSC activation and liver fibrosis. Nucleic Acids Research, 2022, 50, 2440-2451.	14.5	8
121	Synthesis of polysubstituted Î²-amino cyclohexane carboxylic acids via Dielsâ€“Alder reaction using Ni(II)-complex stabilized Î²-alanine derived dienes. Amino Acids, 2013, 44, 791-796.	2.7	7
122	Synthesis and Biological Evaluation of Novel Isopropanolamine Derivatives as Non-peptide Human Immunodeficiency Virus Protease Inhibitors. Chemical and Pharmaceutical Bulletin, 2008, 56, 1147-1152.	1.3	6
123	Regioselective synthesis of substituted thiazoles via cascade reactions from 3-chlorochromones and thioamides. Organic and Biomolecular Chemistry, 2020, 18, 6162-6170.	2.8	6
124	Steered molecular dynamics simulations of protein-ligand interactions. Science in China Series B: Chemistry, 2004, 47, 355-366.	0.8	5
125	Utilization of 3â€²-carboxy-containing tyrosine derivatives as a new class of phosphotyrosyl mimetics in the preparation of novel non-phosphorylated cyclic peptide inhibitors of the Grb2â€“SH2 domain. Organic and Biomolecular Chemistry, 2006, 4, 659.	2.8	5
126	Identification and Evaluation of Coronavirus Replicase Inhibitors Using a Replicon Cell Line. Advances in Experimental Medicine and Biology, 2006, 581, 609-613.	1.6	3

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127	SOMEViz: A Web Service for Site of Metabolism Estimating and Visualizing. Protein and Peptide Letters, 2012, 19, 905-909.	0.9	2
128	Analysis of Four Types of Leukemia Using Gene Ontology Term and Kyoto Encyclopedia of Genes and Genomes Pathway Enrichment Scores. Combinatorial Chemistry and High Throughput Screening, 2020, 23, 295-303.	1.1	2
129	Identification of novel anti-inflammatory Nur77 modulators by virtual screening. Bioorganic Chemistry, 2021, 112, 104912.	4.1	1
130	Bioactivity Prediction Based on Matched Molecular Pair and Matched Molecular Series Methods. Current Pharmaceutical Design, 2020, 26, 4195-4205.	1.9	1
131	In Silico Prediction of Cytochrome P450-Mediated Site of Metabolism (SOM). Protein and Peptide Letters, 2013, 20, 279-289.	0.9	0