

# Xiaomin Luo

## 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.

133  
papers

5,588  
citations

39  
h-index

70  
g-index

136  
ext. papers

6,417  
ext. citations

5.6  
avg, IF

4.97  
L-index

#	Paper	IF	Citations
133	Active Learning for Drug Design: A Case Study on the Plasma Exposure of Orally Administered Drugs. <i>Journal of Medicinal Chemistry</i> , <b>2021</b> , 64, 16838-16853	8.3	2
132	Hepatoprotective Effect and Potential Mechanism of Aqueous Extract from on Carbon-Tetrachloride-Induced Liver Fibrosis in Rats. <i>Evidence-based Complementary and Alternative Medicine</i> , <b>2021</b> , 2021, 5345821	2.3	3
131	Synthesis, characterization, in vitro antioxidant and hypoglycemic activities of selenium nanoparticles decorated with polysaccharides of <i>Gracilaria lemaneiformis</i> . <i>International Journal of Biological Macromolecules</i> , <b>2021</b> , 193, 923-932	7.9	8
130	Drug repurposing against breast cancer by integrating drug-exposure expression profiles and drug-drug links based on graph neural network. <i>Bioinformatics</i> , <b>2021</b> ,	7.2	8
129	Identification of novel anti-inflammatory Nur77 modulators by virtual screening. <i>Bioorganic Chemistry</i> , <b>2021</b> , 112, 104912	5.1	0
128	Discovery of Cyclic Peptidomimetic Ligands Targeting the Extracellular Domain of EGFR. <i>Journal of Medicinal Chemistry</i> , <b>2021</b> , 64, 11219-11228	8.3	0
127	A hybrid framework for improving uncertainty quantification in deep learning-based QSAR regression modeling. <i>Journal of Cheminformatics</i> , <b>2021</b> , 13, 69	8.6	0
126	Revisiting Aldehyde Oxidase Mediated Metabolism in Drug-like Molecules: An Improved Computational Model. <i>Journal of Medicinal Chemistry</i> , <b>2020</b> , 63, 6523-6537	8.3	3
125	Diterpenoids from the Root Bark of and Evaluation of Their Phosphodiesterase Type 4D Inhibitory Activity. <i>Journal of Natural Products</i> , <b>2020</b> , 83, 1229-1237	4.9	2
124	Analysis of Four Types of Leukemia Using Gene Ontology Term and Kyoto Encyclopedia of Genes and Genomes Pathway Enrichment Scores. <i>Combinatorial Chemistry and High Throughput Screening</i> , <b>2020</b> , 23, 295-303	1.3	1
123	Bioactivity Prediction Based on Matched Molecular Pair and Matched Molecular Series Methods. <i>Current Pharmaceutical Design</i> , <b>2020</b> , 26, 4195-4205	3.3	0
122	TransformerCPI: improving compound-protein interaction prediction by sequence-based deep learning with self-attention mechanism and label reversal experiments. <i>Bioinformatics</i> , <b>2020</b> , 36, 4406-4414	7.2	41
121	Regioselective synthesis of substituted thiazoles via cascade reactions from 3-chlorochromones and thioamides. <i>Organic and Biomolecular Chemistry</i> , <b>2020</b> , 18, 6162-6170	3.9	2
120	Machine-Learning-Guided Cocrystal Prediction Based on Large Data Base. <i>Crystal Growth and Design</i> , <b>2020</b> , 20, 6610-6621	3.5	11
119	Pushing the Boundaries of Molecular Representation for Drug Discovery with the Graph Attention Mechanism. <i>Journal of Medicinal Chemistry</i> , <b>2020</b> , 63, 8749-8760	8.3	93
118	Deep Neural Network Classifier for Virtual Screening Inhibitors of (S)-Adenosyl-L-Methionine (SAM)-Dependent Methyltransferase Family. <i>Frontiers in Chemistry</i> , <b>2019</b> , 7, 324	5	5
117	Computational chemical biology and drug design: Facilitating protein structure, function, and modulation studies. <i>Medicinal Research Reviews</i> , <b>2018</b> , 38, 914-950	14.4	23

116	Machine Learning-Based Modeling of Drug Toxicity. <i>Methods in Molecular Biology</i> , <b>2018</b> , 1754, 247-264	1.4	10
115	Aldehyde Oxidase Mediated Metabolism in Drug-like Molecules: A Combined Computational and Experimental Study. <i>Journal of Medicinal Chemistry</i> , <b>2017</b> , 60, 2973-2982	8.3	29
114	Identification and biochemical characterization of DC07090 as a novel potent small molecule inhibitor against human enterovirus 71 3C protease by structure-based virtual screening. <i>European Journal of Medicinal Chemistry</i> , <b>2016</b> , 124, 981-991	6.8	19
113	Estimation of elimination half-lives of organic chemicals in humans using gradient boosting machine. <i>Biochimica Et Biophysica Acta - General Subjects</i> , <b>2016</b> , 1860, 2664-71	4	19
112	Discovery of Novel Inhibitors Targeting the Menin-Mixed Lineage Leukemia Interface Using Pharmacophore- and Docking-Based Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , <b>2016</b> , 56, 1847-55	6.1	19
111	TarPred: a web application for predicting therapeutic and side effect targets of chemical compounds. <i>Bioinformatics</i> , <b>2015</b> , 31, 2049-51	7.2	29
110	Policresulen, a novel NS2B/NS3 protease inhibitor, effectively inhibits the replication of DENV2 virus in BHK-21 cells. <i>Acta Pharmacologica Sinica</i> , <b>2015</b> , 36, 1126-36	8	21
109	Combinatorial Pharmacophore Modeling of Multidrug and Toxin Extrusion Transporter 1 Inhibitors: a Theoretical Perspective for Understanding Multiple Inhibitory Mechanisms. <i>Scientific Reports</i> , <b>2015</b> , 5, 13684	4.9	11
108	In silico ADME/T modelling for rational drug design. <i>Quarterly Reviews of Biophysics</i> , <b>2015</b> , 48, 488-515	7	137
107	Identification of novel thiadiazoloacrylamide analogues as inhibitors of dengue-2 virus NS2B/NS3 protease. <i>Bioorganic and Medicinal Chemistry</i> , <b>2014</b> , 22, 6344-52	3.4	28
106	In silico site of metabolism prediction for human UGT-catalyzed reactions. <i>Bioinformatics</i> , <b>2014</b> , 30, 398-405	4.05	23
105	Estimation of acute oral toxicity in rat using local lazy learning. <i>Journal of Cheminformatics</i> , <b>2014</b> , 6, 26	8.6	25
104	Mechanism of the All- $\beta$ to All- $\alpha$ Conformational Transition of RfaH-CTD: Molecular Dynamics Simulation and Markov State Model. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 2255-64	6.4	24
103	Thermodynamic and structural characterization of halogen bonding in protein-ligand interactions: a case study of PDE5 and its inhibitors. <i>Journal of Medicinal Chemistry</i> , <b>2014</b> , 57, 3588-93	8.3	28
102	Novel Bayesian classification models for predicting compounds blocking hERG potassium channels. <i>Acta Pharmacologica Sinica</i> , <b>2014</b> , 35, 1093-102	8	39
101	In Silico target fishing: addressing a "Big Data" problem by ligand-based similarity rankings with data fusion. <i>Journal of Cheminformatics</i> , <b>2014</b> , 6, 33	8.6	35
100	Synthesis of polysubstituted $\beta$ -amino cyclohexane carboxylic acids via Diels-Alder reaction using Ni(II)-complex stabilized $\beta$ -alanine derived dienes. <i>Amino Acids</i> , <b>2013</b> , 44, 791-6	3.5	7
99	Identification of novel small molecules as inhibitors of hepatitis C virus by structure-based virtual screening. <i>International Journal of Molecular Sciences</i> , <b>2013</b> , 14, 22845-56	6.3	10

98	Binding sensitivity of adefovir to the polymerase from different genotypes of HBV: molecular modeling, docking and dynamics simulation studies. <i>Acta Pharmacologica Sinica</i> , <b>2013</b> , 34, 319-28	8	9
97	Identification of 15d-PGJ2 as an antagonist of farnesoid X receptor: molecular modeling with biological evaluation. <i>Steroids</i> , <b>2013</b> , 78, 813-22	2.8	16
96	Combinatorial pharmacophore modeling of organic cation transporter 2 (OCT2) inhibitors: insights into multiple inhibitory mechanisms. <i>Molecular Pharmaceutics</i> , <b>2013</b> , 10, 4611-9	5.6	17
95	In Silico Prediction of Cytochrome P450-Mediated Site of Metabolism (SOM). <i>Protein and Peptide Letters</i> , <b>2013</b> , 20, 279-289	1.9	
94	Computational models for predicting interactions with membrane transporters. <i>Current Medicinal Chemistry</i> , <b>2013</b> , 20, 2118-36	4.3	8
93	Non-covalent interactions with aromatic rings: current understanding and implications for rational drug design. <i>Current Pharmaceutical Design</i> , <b>2013</b> , 19, 6522-33	3.3	24
92	A novel sulfonamide agent, MPSP-001, exhibits potent activity against human cancer cells in vitro through disruption of microtubule. <i>Acta Pharmacologica Sinica</i> , <b>2012</b> , 33, 261-70	8	25
91	Estimation of carcinogenicity using molecular fragments tree. <i>Journal of Chemical Information and Modeling</i> , <b>2012</b> , 52, 1994-2003	6.1	14
90	Conformational transition and energy landscape of ErbB4 activated by neuregulin1 alone microsecond molecular dynamics simulations. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 6720-31	16.4	19
89	Discovery of novel dual-action antidiabetic agents that inhibit glycogen phosphorylase and activate glucokinase. <i>European Journal of Medicinal Chemistry</i> , <b>2012</b> , 58, 624-39	6.8	16
88	SOMEViz: a web service for site of metabolism estimating and visualizing. <i>Protein and Peptide Letters</i> , <b>2012</b> , 19, 905-9	1.9	1
87	Computational Approaches to Drug Discovery and Development <b>2012</b> , 23-40		1
86	Knowledge-based scoring functions in drug design: 3. A two-dimensional knowledge-based hydrogen-bonding potential for the prediction of protein-ligand interactions. <i>Journal of Chemical Information and Modeling</i> , <b>2011</b> , 51, 2994-3004	6.1	14
85	Computational screening for active compounds targeting protein sequences: methodology and experimental validation. <i>Journal of Chemical Information and Modeling</i> , <b>2011</b> , 51, 2821-8	6.1	48
84	Fragment-based prediction of skin sensitization using recursive partitioning. <i>Journal of Computer-Aided Molecular Design</i> , <b>2011</b> , 25, 885-93	4.2	9
83	Knowledge-based scoring functions in drug design: 2. Can the knowledge base be enriched?. <i>Journal of Chemical Information and Modeling</i> , <b>2011</b> , 51, 386-97	6.1	25
82	Design, synthesis, and interaction study of quinazoline-2(1H)-thione derivatives as novel potential Bcl-xL inhibitors. <i>Journal of Medicinal Chemistry</i> , <b>2010</b> , 53, 3465-79	8.3	39
81	Using support vector regression coupled with the genetic algorithm for predicting acute toxicity to the fathead minnow. <i>SAR and QSAR in Environmental Research</i> , <b>2010</b> , 21, 559-70	3.5	32

80	Molecular dynamics simulations on the mechanism of transporting methylamine and ammonia by ammonium transporter AmtB. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 15172-9	3.4	19
79	Novel thiophene derivatives as PTP1B inhibitors with selectivity and cellular activity. <i>Bioorganic and Medicinal Chemistry</i> , <b>2010</b> , 18, 1773-82	3.4	54
78	Site of metabolism prediction for six biotransformations mediated by cytochromes P450. <i>Bioinformatics</i> , <b>2009</b> , 25, 1251-8	7.2	61
77	Interaction models of a series of oxadiazole-substituted alpha-isopropoxy phenylpropanoic acids against PPARalpha and PPARgamma: molecular modeling and comparative molecular similarity indices analysis studies. <i>Protein and Peptide Letters</i> , <b>2009</b> , 16, 150-62	1.9	11
76	Pharmacophore-based virtual screening versus docking-based virtual screening: a benchmark comparison against eight targets. <i>Acta Pharmacologica Sinica</i> , <b>2009</b> , 30, 1694-708	8	68
75	Halogen bonding--a novel interaction for rational drug design?. <i>Journal of Medicinal Chemistry</i> , <b>2009</b> , 52, 2854-62	8.3	485
74	Efficient synthesis of alpha-aryl-/heteroaryl-substituted beta-amino acids via Ni(II) complex through the Suzuki coupling reaction. <i>Journal of Organic Chemistry</i> , <b>2009</b> , 74, 5656-9	4.2	12
73	C-X...H contacts in biomolecular systems: how they contribute to protein-ligand binding affinity. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 12615-21	3.4	80
72	PDTD: a web-accessible protein database for drug target identification. <i>BMC Bioinformatics</i> , <b>2008</b> , 9, 104	3.6	205
71	An improved PMF scoring function for universally predicting the interactions of a ligand with protein, DNA, and RNA. <i>Journal of Chemical Information and Modeling</i> , <b>2008</b> , 48, 1438-47	6.1	37
70	Dynamic mechanism of fatty acid transport across cellular membranes through FadL: molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 13070-8	3.4	10
69	Synthesis and biological evaluation of novel isopropanolamine derivatives as non-peptide human immunodeficiency virus protease inhibitors. <i>Chemical and Pharmaceutical Bulletin</i> , <b>2008</b> , 56, 1147-52	1.9	3
68	Drug Discovery and Development: Computational Approaches <b>2008</b> , 1		2
67	Research progress in cation- $\pi$ interactions. <i>Science in China Series B: Chemistry</i> , <b>2008</b> , 51, 709-717		23
66	Tryptophan-containing dipeptide derivatives as potent PPARgamma antagonists: design, synthesis, biological evaluation, and molecular modeling. <i>European Journal of Medicinal Chemistry</i> , <b>2008</b> , 43, 2699-716	6.8	12
65	Discovering novel 3-nitroquinolines as a new class of anticancer agents. <i>Acta Pharmacologica Sinica</i> , <b>2008</b> , 29, 1529-38	8	21
64	Molecular insight into the interaction between IFABP and PA by using MM-PBSA and alanine scanning methods. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 9104-13	3.4	15
63	Dopamine D1 receptor agonist and D2 receptor antagonist effects of the natural product (-)-stepholidine: molecular modeling and dynamics simulations. <i>Biophysical Journal</i> , <b>2007</b> , 93, 1431-41	2.9	33

62	Indole derivatives as potent inhibitors of 5-lipoxygenase: design, synthesis, biological evaluation, and molecular modeling. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2007</b> , 17, 2414-20	2.9	27
61	Understanding the regulation mechanisms of PAF receptor by agonists and antagonists: molecular modeling and molecular dynamics simulation studies. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2007</b> , 67, 41-52	4.2	17
60	3D-QSAR study of 20 (S)-camptothecin analogs. <i>Acta Pharmacologica Sinica</i> , <b>2007</b> , 28, 307-14	8	13
59	Pharmacophore-directed homology modeling and molecular dynamics simulation of G protein-coupled receptor: study of possible binding modes of 5-HT <sub>2C</sub> receptor agonists. <i>Acta Biochimica Et Biophysica Sinica</i> , <b>2007</b> , 39, 413-22	2.8	10
58	Predicting protein-protein interactions based only on sequences information. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2007</b> , 104, 4337-41	11.5	593
57	Possible pathway(s) of metyrapone egress from the active site of cytochrome P450 3A4: a molecular dynamics simulation. <i>Drug Metabolism and Disposition</i> , <b>2007</b> , 35, 689-96	4	49
56	Discovering potassium channel blockers from synthetic compound database by using structure-based virtual screening in conjunction with electrophysiological assay. <i>Journal of Medicinal Chemistry</i> , <b>2007</b> , 50, 83-93	8.3	26
55	Molecular dynamics of nicotinic acetylcholine receptor correlating biological functions. <i>Current Protein and Peptide Science</i> , <b>2006</b> , 7, 195-200	2.8	10
54	Mutagenic probability estimation of chemical compounds by a novel molecular electrophilicity vector and support vector machine. <i>Bioinformatics</i> , <b>2006</b> , 22, 2099-106	7.2	25
53	TarFisDock: a web server for identifying drug targets with docking approach. <i>Nucleic Acids Research</i> , <b>2006</b> , 34, W219-24	20.1	313
52	Binding investigation of human 5-lipoxygenase with its inhibitors by SPR technology correlating with molecular docking simulation. <i>Journal of Biochemistry</i> , <b>2006</b> , 139, 715-23	3.1	29
51	Design, synthesis and antitumor evaluation of a new series of N-substituted-thiourea derivatives. <i>Acta Pharmacologica Sinica</i> , <b>2006</b> , 27, 1259-71	8	19
50	Utilization of 3Qcarboxy-containing tyrosine derivatives as a new class of phosphotyrosyl mimetics in the preparation of novel non-phosphorylated cyclic peptide inhibitors of the Grb2-SH2 domain. <i>Organic and Biomolecular Chemistry</i> , <b>2006</b> , 4, 659-66	3.9	5
49	Strategy for discovering chemical inhibitors of human cyclophilin a: focused library design, virtual screening, chemical synthesis and bioassay. <i>ACS Combinatorial Science</i> , <b>2006</b> , 8, 326-37		36
48	Blocking of the nicotinic acetylcholine receptor ion channel by chlorpromazine, a noncompetitive inhibitor: A molecular dynamics simulation study. <i>Journal of Physical Chemistry B</i> , <b>2006</b> , 110, 20640-8	3.4	16
47	Molecular dynamics simulations of interaction between protein-tyrosine phosphatase 1B and a bidentate inhibitor. <i>Acta Pharmacologica Sinica</i> , <b>2006</b> , 27, 100-10	8	20
46	Paeoniflorin attenuates neuroinflammation and dopaminergic neurodegeneration in the MPTP model of Parkinson's disease by activation of adenosine A1 receptor. <i>British Journal of Pharmacology</i> , <b>2006</b> , 148, 314-25	8.6	97
45	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. <i>Bioorganic and Medicinal Chemistry</i> , <b>2006</b> , 14, 3428-37	3.4	19

44	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. <i>Journal of Computer-Aided Molecular Design</i> , <b>2006</b> , 20, 281-93	4.2	13
43	QSAR analyses on avian influenza virus neuraminidase inhibitors using CoMFA, CoMSIA, and HQSAR. <i>Journal of Computer-Aided Molecular Design</i> , <b>2006</b> , 20, 549-66	4.2	16
42	Identification and evaluation of coronavirus replicase inhibitors using a replicon cell line. <i>Advances in Experimental Medicine and Biology</i> , <b>2006</b> , 581, 609-13	3.6	3
41	Focused combinatorial library design based on structural diversity, druglikeness and binding affinity score. <i>ACS Combinatorial Science</i> , <b>2005</b> , 7, 398-406		61
40	A new rapid and effective chemistry space filter in recognizing a druglike database. <i>Journal of Chemical Information and Modeling</i> , <b>2005</b> , 45, 856-62	6.1	60
39	Dynamic mechanism for the autophosphorylation of CheA histidine kinase: molecular dynamics simulations. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 11709-19	16.4	28
38	Expression and purification of the catalytic domain of human vascular endothelial growth factor receptor 2 for inhibitor screening. <i>Biochimica Et Biophysica Acta - General Subjects</i> , <b>2005</b> , 1722, 254-61	4	11
37	Dynamic mechanism of E2020 binding to acetylcholinesterase: a steered molecular dynamics simulation. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 23730-8	3.4	47
36	Influence of the water molecule on cation-pi interaction: ab initio second order Møller-Plesset perturbation theory (MP2) calculations. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 5945-9	3.4	43
35	Conformational dynamics of the nicotinic acetylcholine receptor channel: a 35-ns molecular dynamics simulation study. <i>Journal of the American Chemical Society</i> , <b>2005</b> , 127, 1291-9	16.4	61
34	QSAR analyses on ginkgolides and their analogues using CoMFA, CoMSIA, and HQSAR. <i>Bioorganic and Medicinal Chemistry</i> , <b>2005</b> , 13, 313-22	3.4	28
33	Molecular docking and 3D-QSAR studies on the binding mechanism of statine-based peptidomimetics with beta-secretase. <i>Bioorganic and Medicinal Chemistry</i> , <b>2005</b> , 13, 2121-31	3.4	28
32	Synthesis and antitumor evaluation of novel 5-substituted-4-hydroxy-8-nitroquinazolines as EGFR signaling-targeted inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , <b>2005</b> , 13, 5613-22	3.4	35
31	Computational analysis of molecular basis of 1:1 interactions of NRG-1beta wild-type and variants with ErbB3 and ErbB4. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2005</b> , 59, 742-56	4.2	21
30	Conformational transition of amyloid beta-peptide. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2005</b> , 102, 5403-7	11.5	222
29	Cinanserin is an inhibitor of the 3C-like proteinase of severe acute respiratory syndrome coronavirus and strongly reduces virus replication in vitro. <i>Journal of Virology</i> , <b>2005</b> , 79, 7095-103	6.6	156
28	Possible pathway(s) of testosterone egress from the active site of cytochrome P450 2B1: a steered molecular dynamics simulation. <i>Drug Metabolism and Disposition</i> , <b>2005</b> , 33, 910-9	4	45
27	Steered molecular dynamics simulations of protein-ligand interactions. <i>Science in China Series B: Chemistry</i> , <b>2004</b> , 47, 355-366		4

26	GasDock: a new approach for rapid flexible docking based on an improved multi-population genetic algorithm. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2004</b> , 14, 4671-6	2.9	51
25	Elucidating inhibitory models of the inhibitors of epidermal growth factor receptor by docking and 3D-QSAR. <i>Bioorganic and Medicinal Chemistry</i> , <b>2004</b> , 12, 2409-17	3.4	16
24	Inhibitory mode of indole-2-carboxamide derivatives against HLGPa: molecular docking and 3D-QSAR analyses. <i>Bioorganic and Medicinal Chemistry</i> , <b>2004</b> , 12, 4147-57	3.4	21
23	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. <i>Bioorganic and Medicinal Chemistry</i> , <b>2004</b> , 12, 6193-208	3.4	47
22	Computational simulations of interactions of scorpion toxins with the voltage-gated potassium ion channel. <i>Biophysical Journal</i> , <b>2004</b> , 86, 3542-55	2.9	54
21	Nucleocapsid protein of SARS coronavirus tightly binds to human cyclophilin A. <i>Biochemical and Biophysical Research Communications</i> , <b>2004</b> , 321, 557-65	3.4	92
20	Simulating the interactions of toxins with K <sup>+</sup> channels. <i>Current Pharmaceutical Design</i> , <b>2004</b> , 10, 1057-67	3.3	13
19	Virtual screening on natural products for discovering active compounds and target information. <i>Current Medicinal Chemistry</i> , <b>2003</b> , 10, 2327-42	4.3	102
18	Progress in clinical, pharmacological, chemical and structural biological studies of huperzine A: a drug of traditional chinese medicine origin for the treatment of Alzheimer's disease. <i>Current Medicinal Chemistry</i> , <b>2003</b> , 10, 2231-52	4.3	95
17	Structure-based discovery of potassium channel blockers from natural products: virtual screening and electrophysiological assay testing. <i>Chemistry and Biology</i> , <b>2003</b> , 10, 1103-13		44
16	N-methylformamide-benzene complex as a prototypical peptide N-H... $\pi$ hydrogen-bonded system: density functional theory and MP2 studies. <i>Journal of Organic Chemistry</i> , <b>2003</b> , 68, 7490-5	4.2	25
15	How does huperzine A enter and leave the binding gorge of acetylcholinesterase? Steered molecular dynamics simulations. <i>Journal of the American Chemical Society</i> , <b>2003</b> , 125, 11340-9	16.4	87
14	Molecular dynamics simulations on SDF-1 $\alpha$ : binding with CXCR4 receptor. <i>Biophysical Journal</i> , <b>2003</b> , 84, 171-84	2.9	61
13	Steered molecular dynamics simulation on the binding of NNRTI to HIV-1 RT. <i>Biophysical Journal</i> , <b>2003</b> , 84, 3547-63	2.9	72
12	Molecular docking and 3-D-QSAR studies on the possible antimalarial mechanism of artemisinin analogues. <i>Bioorganic and Medicinal Chemistry</i> , <b>2002</b> , 10, 2883-91	3.4	53
11	Molecular docking and 3D-QSAR studies on gag peptide analogue inhibitors interacting with human cyclophilin A. <i>Journal of Medicinal Chemistry</i> , <b>2002</b> , 45, 5249-59	8.3	20
10	Elucidating the inhibiting mode of AHPBA derivatives against HIV-1 protease and building predictive 3D-QSAR models. <i>Journal of Medicinal Chemistry</i> , <b>2002</b> , 45, 333-43	8.3	38
9	A density-functional study of the mechanism for the diastereoselective epoxidation of chiral allylic alcohols by the titanium peroxy complexes. <i>Journal of Organic Chemistry</i> , <b>2002</b> , 67, 1427-35	4.2	23



8	Inhibitory mode of 1,5-diarylpyrazole derivatives against cyclooxygenase-2 and cyclooxygenase-1: molecular docking and 3D QSAR analyses. <i>Journal of Medicinal Chemistry</i> , <b>2002</b> , 45, 4816-27	8.3	58
7	New p-methylsulfonamido phenylethylamine analogues as class III antiarrhythmic agents: design, synthesis, biological assay, and 3D-QSAR analysis. <i>Journal of Medicinal Chemistry</i> , <b>2002</b> , 45, 2953-69	8.3	18
6	Brownian dynamics simulations of the recognition of the scorpion toxin P05 with the small-conductance calcium-activated potassium channels. <i>Journal of Molecular Biology</i> , <b>2002</b> , 318, 417-28	6.5	43
5	Steered molecular dynamics simulations on the "tail helix latch" hypothesis in the gelsolin activation process. <i>Biophysical Journal</i> , <b>2002</b> , 83, 753-62	2.9	12
4	Brownian dynamics simulations of the recognition of the scorpion toxin maurotoxin with the voltage-gated potassium ion channels. <i>Biophysical Journal</i> , <b>2002</b> , 83, 2370-85	2.9	46
3	3D-QSAR model of flavonoids binding at benzodiazepine site in GABAA receptors. <i>Journal of Medicinal Chemistry</i> , <b>2001</b> , 44, 1883-91	8.3	66
2	Brownian dynamics simulations of interaction between scorpion toxin Lq2 and potassium ion channel. <i>Biophysical Journal</i> , <b>2001</b> , 80, 1659-69	2.9	40
1	Computational target fishing by mining transcriptional data using a novel Siamese spectral-based graph convolutional network		2