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	Small molecule targeting CELF1 RNA-binding activity to control HSC activation and liver fibrosis. Nucleic Acids Research, 2022, 50, 2440-2451.	14.5	8
2	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
3	Identification of novel anti-inflammatory Nur77 modulators by virtual screening. Bioorganic Chemistry, 2021, 112, 104912.	4.1	1
4	Discovery of Cyclic Peptidomimetic Ligands Targeting the Extracellular Domain of EGFR. Journal of Medicinal Chemistry, 2021, 64, 11219-11228.	6.4	9
5	A hybrid framework for improving uncertainty quantification in deep learning-based QSAR regression modeling. Journal of Cheminformatics, 2021, 13, 69.	6.1	18
6	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
7	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
8	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
9	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
10	Regioselective synthesis of substituted thiazoles via cascade reactions from 3-chlorochromones and thioamides. Organic and Biomolecular Chemistry, 2020, 18, 6162-6170.	2.8	6
11	Machine-Learning-Guided Cocrystal Prediction Based on Large Data Base. Crystal Growth and Design, 2020, 20, 6610-6621.	3.0	38
12	Revisiting Aldehyde Oxidase Mediated Metabolism in Drug-like Molecules: An Improved Computational Model. Journal of Medicinal Chemistry, 2020, 63, 6523-6537.	6.4	10
13	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
14	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
15	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
16	Bioactivity Prediction Based on Matched Molecular Pair and Matched Molecular Series Methods. Current Pharmaceutical Design, 2020, 26, 4195-4205.	1.9	1
17	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
18	Computational chemical biology and drug design: Facilitating protein structure, function, and modulation studies. Medicinal Research Reviews, 2018, 38, 914-950.	10.5	38

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19	Machine Learning-Based Modeling of Drug Toxicity. Methods in Molecular Biology, 2018, 1754, 247-264.	0.9	14
20	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
21	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
22	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
23	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
24	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
25	In silicoADME/T modelling for rational drug design. Quarterly Reviews of Biophysics, 2015, 48, 488-515.	5.7	250
26	TarPred: a web application for predicting therapeutic and side effect targets of chemical compounds. Bioinformatics, 2015, 31, 2049-2051.	4.1	52
27	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
28	Novel Bayesian classification models for predicting compounds blocking hERG potassium channels. Acta Pharmacologica Sinica, 2014, 35, 1093-1102.	6.1	53
29	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
30	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
31	In silico site of metabolism prediction for human UGT-catalyzed reactions. Bioinformatics, 2014, 30, 398-405.	4.1	29
32	Estimation of acute oral toxicity in rat using local lazy learning. Journal of Cheminformatics, 2014, 6, 26.	6.1	30
33	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
34	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
35	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
36	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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37	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
38	Identification of 15d-PGJ2 as an antagonist of farnesoid X receptor: Molecular modeling with biological evaluation. Steroids, 2013, 78, 813-822.	1.8	20
39	Combinatorial Pharmacophore Modeling of Organic Cation Transporter 2 (OCT2) Inhibitors: Insights into Multiple Inhibitory Mechanisms. Molecular Pharmaceutics, 2013, 10, 4611-4619.	4.6	21
40	In Silico Prediction of Cytochrome P450-Mediated Site of Metabolism (SOM). Protein and Peptide Letters, 2013, 20, 279-289.	0.9	0
41	Computational Models for Predicting Interactions with Membrane Transporters. Current Medicinal Chemistry, 2013, 20, 2118-2136.	2.4	8
42	Non-Covalent Interactions with Aromatic Rings: Current Understanding and Implications for Rational Drug Design. Current Pharmaceutical Design, 2013, 19, 6522-6533.	1.9	33
43	SOMEViz: A Web Service for Site of Metabolism Estimating and Visualizing. Protein and Peptide Letters, 2012, 19, 905-909.	0.9	2
44	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
45	Estimation of Carcinogenicity Using Molecular Fragments Tree. Journal of Chemical Information and Modeling, 2012, 52, 1994-2003.	5.4	15
46	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
47	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
48	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
49	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
50	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
51	Fragment-based prediction of skin sensitization using recursive partitioning. Journal of Computer-Aided Molecular Design, 2011, 25, 885-893.	2.9	10
52	Novel thiophene derivatives as PTP1B inhibitors with selectivity and cellular activity. Bioorganic and Medicinal Chemistry, 2010, 18, 1773-1782.	3.0	59
53	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
54	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

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55	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
56	Site of metabolism prediction for six biotransformations mediated by cytochromes P450. Bioinformatics, 2009, 25, 1251-1258.	4.1	72
57	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
58	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
59	Halogen Bondingâ€"A Novel Interaction for Rational Drug Design?. Journal of Medicinal Chemistry, 2009, 52, 2854-2862.	6.4	524
60	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
61	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
62	Research progress in cation-Ï€ interactions. Science in China Series B: Chemistry, 2008, 51, 709-717.	0.8	24
63	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
64	Discovering novel 3-nitroquinolines as a new class of anticancer agents. Acta Pharmacologica Sinica, 2008, 29, 1529-1538.	6.1	23
65	PDTD: a web-accessible protein database for drug target identification. BMC Bioinformatics, 2008, 9, 104.	2.6	249
66	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
67	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
68	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
69	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
70	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
71	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
72	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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73	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
74	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
75	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
76	3D-QSAR study of 20 (S)-camptothecin analogs. Acta Pharmacologica Sinica, 2007, 28, 307-314.	6.1	18
77	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
78	TarFisDock: a web server for identifying drug targets with docking approach. Nucleic Acids Research, 2006, 34, W219-W224.	14.5	372
79	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
80	Design, synthesis and antitumor evaluation of a new series of N-substituted-thiourea derivatives. Acta Pharmacologica Sinica, 2006, 27, 1259-1271.	6.1	26
81	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
82	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
83	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
84	Molecular dynamics simulations of interaction between protein-tyrosine phosphatase 1B and a bidentate inhibitor1. Acta Pharmacologica Sinica, 2006, 27, 100-110.	6.1	23
85	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
86	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
87	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
88	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
89	Molecular Dynamics of Nicotinic Acetylcholine Receptor Correlating Biological Functions. Current Protein and Peptide Science, 2006, 7, 195-200.	1.4	11
90	Mutagenic probability estimation of chemical compounds by a novel molecular electrophilicity vector and support vector machine. Bioinformatics, 2006, 22, 2099-2106.	4.1	28

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91	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
92	QSAR analyses on ginkgolides and their analogues using CoMFA, CoMSIA, and HQSAR. Bioorganic and Medicinal Chemistry, 2005, 13, 313-322.	3.0	33
93	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
94	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
95	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
96	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
97	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
98	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
99	Focused Combinatorial Library Design Based on Structural Diversity, Druglikeness and Binding Affinity Score. ACS Combinatorial Science, 2005, 7, 398-406.	3.3	69
100	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
101	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
102	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
103	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
104	Influence of the Water Molecule on Cationâˆ'Ï€ Interaction:Â Ab Initio Second Order MÃ¸llerâˆ'Plesset Perturbation Theory (MP2) Calculations. Journal of Physical Chemistry B, 2005, 109, 5945-5949.	2.6	46
105	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
106	Steered molecular dynamics simulations of protein-ligand interactions. Science in China Series B: Chemistry, 2004, 47, 355-366.	0.8	5
107	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
108	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

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109	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
110	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
111	Computational Simulations of Interactions of Scorpion Toxins with the Voltage-Gated Potassium Ion Channel. Biophysical Journal, 2004, 86, 3542-3555.	0.5	55
112	Nucleocapsid protein of SARS coronavirus tightly binds to human cyclophilin A. Biochemical and Biophysical Research Communications, 2004, 321, 557-565.	2.1	104
113	Simulating the Interactions of Toxins with K+ Channels. Current Pharmaceutical Design, 2004, 10, 1057-1067.	1.9	14
114	Structure-Based Discovery of Potassium Channel Blockers from Natural Products. Chemistry and Biology, 2003, 10, 1103-1113.	6.0	50
115	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
116	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
117	Molecular Dynamics Simulations on SDF-1Î±: Binding with CXCR4 Receptor. Biophysical Journal, 2003, 84, 171-184.	0.5	67
118	Steered Molecular Dynamics Simulation on the Binding of NNRTI to HIV-1 RT. Biophysical Journal, 2003, 84, 3547-3563.	0.5	77
119	Virtual Screening on Natural Products for Discovering Active Compounds and Target Information. Current Medicinal Chemistry, 2003, 10, 2327-2342.	2.4	123
120	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
121	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
122	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
123	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
124	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
125	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
126	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

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127	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
128	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
129	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
130	3D-QSAR Model of Flavonoids Binding at Benzodiazepine Site in GABAA Receptors. Journal of Medicinal Chemistry, 2001, 44, 1883-1891.	6.4	75
131	Brownian Dynamics Simulations of Interaction Between Scorpion Toxin Lq2 and Potassium Ion Channel. Biophysical Journal, 2001, 80, 1659-1669.	0.5	42