Xiaomin Luo

List of Publications by Citations

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	Predicting protein-protein interactions based only on sequences information. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 4337-41	11.5	593
132	Halogen bonding--a novel interaction for rational drug design?. *Journal of Medicinal Chemistry*, **2009**, 52, 2854-62	8.3	485
131	TarFisDock: a web server for identifying drug targets with docking approach. *Nucleic Acids Research*, **2006**, 34, W219-24	20.1	313
130	Conformational transition of amyloid beta-peptide. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 5403-7	11.5	222
129	PDTD: a web-accessible protein database for drug target identification. *BMC Bioinformatics*, **2008**, 9, 104	3.6	205
128	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, 7095-103	6.6	156
127	In silico ADME/T modelling for rational drug design. *Quarterly Reviews of Biophysics*, **2015**, 48, 488-515	7	137
126	Virtual screening on natural products for discovering active compounds and target information. *Current Medicinal Chemistry*, **2003**, 10, 2327-42	4.3	102
125	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, 314-25	8.6	97
124	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. *Current Medicinal Chemistry*, **2003**, 10, 2231-52	4.3	95
123	Pushing the Boundaries of Molecular Representation for Drug Discovery with the Graph Attention Mechanism. *Journal of Medicinal Chemistry*, **2020**, 63, 8749-8760	8.3	93
122	Nucleocapsid protein of SARS coronavirus tightly binds to human cyclophilin A. *Biochemical and Biophysical Research Communications*, **2004**, 321, 557-65	3.4	92
121	How does huperzine A enter and leave the binding gorge of acetylcholinesterase? Steered molecular dynamics simulations. *Journal of the American Chemical Society*, **2003**, 125, 11340-9	16.4	87
120	C-X...H contacts in biomolecular systems: how they contribute to protein-ligand binding affinity. *Journal of Physical Chemistry B*, **2009**, 113, 12615-21	3.4	80
119	Steered molecular dynamics simulation on the binding of NNRTI to HIV-1 RT. *Biophysical Journal*, **2003**, 84, 3547-63	2.9	72
118	Pharmacophore-based virtual screening versus docking-based virtual screening: a benchmark comparison against eight targets. *Acta Pharmacologica Sinica*, **2009**, 30, 1694-708	8	68
117	3D-QSAR model of flavonoids binding at benzodiazepine site in GABAA receptors. *Journal of Medicinal Chemistry*, **2001**, 44, 1883-91	8.3	66

116	Site of metabolism prediction for six biotransformations mediated by cytochromes P450. *Bioinformatics*, **2009**, 25, 1251-8	7.2	61
115	Focused combinatorial library design based on structural diversity, druglikeness and binding affinity score. *ACS Combinatorial Science*, **2005**, 7, 398-406		61
114	Conformational dynamics of the nicotinic acetylcholine receptor channel: a 35-ns molecular dynamics simulation study. *Journal of the American Chemical Society*, **2005**, 127, 1291-9	16.4	61
113	Molecular dynamics simulations on SDF-1alpha: binding with CXCR4 receptor. *Biophysical Journal*, **2003**, 84, 171-84	2.9	61
112	A new rapid and effective chemistry space filter in recognizing a druglike database. *Journal of Chemical Information and Modeling*, **2005**, 45, 856-62	6.1	60
111	Inhibitory mode of 1,5-diarylpyrazole derivatives against cyclooxygenase-2 and cyclooxygenase-1: molecular docking and 3D QSAR analyses. *Journal of Medicinal Chemistry*, **2002**, 45, 4816-27	8.3	58
110	Novel thiophene derivatives as PTP1B inhibitors with selectivity and cellular activity. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 1773-82	3.4	54
109	Computational simulations of interactions of scorpion toxins with the voltage-gated potassium ion channel. *Biophysical Journal*, **2004**, 86, 3542-55	2.9	54
108	Molecular docking and 3-D-QSAR studies on the possible antimalarial mechanism of artemisinin analogues. *Bioorganic and Medicinal Chemistry*, **2002**, 10, 2883-91	3.4	53
107	GAsDock: a new approach for rapid flexible docking based on an improved multi-population genetic algorithm. *Bioorganic and Medicinal Chemistry Letters*, **2004**, 14, 4671-6	2.9	51
106	Possible pathway(s) of metyrapone egress from the active site of cytochrome P450 3A4: a molecular dynamics simulation. *Drug Metabolism and Disposition*, **2007**, 35, 689-96	4	49
105	Computational screening for active compounds targeting protein sequences: methodology and experimental validation. *Journal of Chemical Information and Modeling*, **2011**, 51, 2821-8	6.1	48
104	Dynamic mechanism of E2020 binding to acetylcholinesterase: a steered molecular dynamics simulation. *Journal of Physical Chemistry B*, **2005**, 109, 23730-8	3.4	47
103	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, 6193-208	3.4	47
102	Brownian dynamics simulations of the recognition of the scorpion toxin maurotoxin with the voltage-gated potassium ion channels. *Biophysical Journal*, **2002**, 83, 2370-85	2.9	46
101	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, 910-9	4	45
100	Structure-based discovery of potassium channel blockers from natural products: virtual screening and electrophysiological assay testing. *Chemistry and Biology*, **2003**, 10, 1103-13		44
99	Influence of the water molecule on cation-pi interaction: ab initio second order Møller-Plesset perturbation theory (MP2) calculations. *Journal of Physical Chemistry B*, **2005**, 109, 5945-9	3.4	43

98	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, 417-28	6.5	43
97	TransformerCPI: improving compound-protein interaction prediction by sequence-based deep learning with self-attention mechanism and label reversal experiments. *Bioinformatics*, **2020**, 36, 4406-4414	7.2	41
96	Brownian dynamics simulations of interaction between scorpion toxin Lq2 and potassium ion channel. *Biophysical Journal*, **2001**, 80, 1659-69	2.9	40
95	Novel Bayesian classification models for predicting compounds blocking hERG potassium channels. *Acta Pharmacologica Sinica*, **2014**, 35, 1093-102	8	39
94	Design, synthesis, and interaction study of quinazoline-2(1H)-thione derivatives as novel potential Bcl-xL inhibitors. *Journal of Medicinal Chemistry*, **2010**, 53, 3465-79	8.3	39
93	Elucidating the inhibiting mode of AHPBA derivatives against HIV-1 protease and building predictive 3D-QSAR models. *Journal of Medicinal Chemistry*, **2002**, 45, 333-43	8.3	38
92	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, 1438-47	6.1	37
91	Strategy for discovering chemical inhibitors of human cyclophilin a: focused library design, virtual screening, chemical synthesis and bioassay. *ACS Combinatorial Science*, **2006**, 8, 326-37		36
90	In Silico target fishing: addressing a "Big Data" problem by ligand-based similarity rankings with data fusion. *Journal of Cheminformatics*, **2014**, 6, 33	8.6	35
89	Synthesis and antitumor evaluation of novel 5-substituted-4-hydroxy-8-nitroquinazolines as EGFR signaling-targeted inhibitors. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 5613-22	3.4	35
88	Dopamine D1 receptor agonist and D2 receptor antagonist effects of the natural product (-)-stepholidine: molecular modeling and dynamics simulations. *Biophysical Journal*, **2007**, 93, 1431-41	2.9	33
87	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, 559-70	3.5	32
86	Aldehyde Oxidase Mediated Metabolism in Drug-like Molecules: A Combined Computational and Experimental Study. *Journal of Medicinal Chemistry*, **2017**, 60, 2973-2982	8.3	29
85	TarPred: a web application for predicting therapeutic and side effect targets of chemical compounds. *Bioinformatics*, **2015**, 31, 2049-51	7.2	29
84	Binding investigation of human 5-lipoxygenase with its inhibitors by SPR technology correlating with molecular docking simulation. *Journal of Biochemistry*, **2006**, 139, 715-23	3.1	29
83	Identification of novel thiadiazoloacrylamide analogues as inhibitors of dengue-2 virus NS2B/NS3 protease. *Bioorganic and Medicinal Chemistry*, **2014**, 22, 6344-52	3.4	28
82	Thermodynamic and structural characterization of halogen bonding in protein-ligand interactions: a case study of PDE5 and its inhibitors. *Journal of Medicinal Chemistry*, **2014**, 57, 3588-93	8.3	28
81	Dynamic mechanism for the autophosphorylation of CheA histidine kinase: molecular dynamics simulations. *Journal of the American Chemical Society*, **2005**, 127, 11709-19	16.4	28

80	QSAR analyses on ginkgolides and their analogues using CoMFA, CoMSIA, and HQSAR. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 313-22	3.4	28
79	Molecular docking and 3D-QSAR studies on the binding mechanism of statine-based peptidomimetics with beta-secretase. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 2121-31	3.4	28
78	Indole derivatives as potent inhibitors of 5-lipoxygenase: design, synthesis, biological evaluation, and molecular modeling. *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 2414-20	2.9	27
77	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	8.3	26
76	Estimation of acute oral toxicity in rat using local lazy learning. *Journal of Cheminformatics*, **2014**, 6, 26	8.6	25
75	A novel sulfonamide agent, MPSP-001, exhibits potent activity against human cancer cells in vitro through disruption of microtubule. *Acta Pharmacologica Sinica*, **2012**, 33, 261-70	8	25
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73	Mutagenic probability estimation of chemical compounds by a novel molecular electrophilicity vector and support vector machine. *Bioinformatics*, **2006**, 22, 2099-106	7.2	25
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71	Mechanism of the All-□to All-□Conformational Transition of RfaH-CTD: Molecular Dynamics Simulation and Markov State Model. *Journal of Chemical Theory and Computation*, **2014**, 10, 2255-64	6.4	24
70	Non-covalent interactions with aromatic rings: current understanding and implications for rational drug design. *Current Pharmaceutical Design*, **2013**, 19, 6522-33	3.3	24
69	Computational chemical biology and drug design: Facilitating protein structure, function, and modulation studies. *Medicinal Research Reviews*, **2018**, 38, 914-950	14.4	23
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67	Research progress in cation-□nteractions. *Science in China Series B: Chemistry*, **2008**, 51, 709-717		23
66	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, 1427-35	4.2	23
65	Policresulen, a novel NS2B/NS3 protease inhibitor, effectively inhibits the replication of DENV2 virus in BHK-21 cells. *Acta Pharmacologica Sinica*, **2015**, 36, 1126-36	8	21
64	Discovering novel 3-nitroquinolines as a new class of anticancer agents. *Acta Pharmacologica Sinica*, **2008**, 29, 1529-38	8	21
63	Inhibitory mode of indole-2-carboxamide derivatives against HLGPa: molecular docking and 3D-QSAR analyses. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 4147-57	3.4	21

62	Computational analysis of molecular basis of 1:1 interactions of NRG-1beta wild-type and variants with ErbB3 and ErbB4. *Proteins: Structure, Function and Bioinformatics*, **2005**, 59, 742-56	4.2	21
61	Molecular dynamics simulations of interaction between protein-tyrosine phosphatase 1B and a bidentate inhibitor. *Acta Pharmacologica Sinica*, **2006**, 27, 100-10	8	20
60	Molecular docking and 3D-QSAR studies on gag peptide analogue inhibitors interacting with human cyclophilin A. *Journal of Medicinal Chemistry*, **2002**, 45, 5249-59	8.3	20
59	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	6.8	19
58	Conformational transition and energy landscape of ErbB4 activated by neuregulin1□one microsecond molecular dynamics simulations. *Journal of the American Chemical Society*, **2012**, 134, 6720-31	16.4	19
57	Molecular dynamics simulations on the mechanism of transporting methylamine and ammonia by ammonium transporter AmtB. *Journal of Physical Chemistry B*, **2010**, 114, 15172-9	3.4	19
56	Design, synthesis and antitumor evaluation of a new series of N-substituted-thiourea derivatives. *Acta Pharmacologica Sinica*, **2006**, 27, 1259-71	8	19
55	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, 3428-37	3.4	19
54	Estimation of elimination half-lives of organic chemicals in humans using gradient boosting machine. *Biochimica Et Biophysica Acta - General Subjects*, **2016**, 1860, 2664-71	4	19
53	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, 1847-55	6.1	19
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50	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	4.2	17
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48	Discovery of novel dual-action antidiabetic agents that inhibit glycogen phosphorylase and activate glucokinase. *European Journal of Medicinal Chemistry*, **2012**, 58, 624-39	6.8	16
47	Blocking of the nicotinic acetylcholine receptor ion channel by chlorpromazine, a noncompetitive inhibitor: A molecular dynamics simulation study. *Journal of Physical Chemistry B*, **2006**, 110, 20640-8	3.4	16
46	QSAR analyses on avian influenza virus neuraminidase inhibitors using CoMFA, CoMSIA, and HQSAR. *Journal of Computer-Aided Molecular Design*, **2006**, 20, 549-66	4.2	16
45	Elucidating inhibitory models of the inhibitors of epidermal growth factor receptor by docking and 3D-QSAR. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 2409-17	3.4	16

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41	3D-QSAR study of 20 (S)-camptothecin analogs. *Acta Pharmacologica Sinica*, **2007**, 28, 307-14	8	13
40	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, 281-93	4.2	13
39	Simulating the interactions of toxins with K+ channels. *Current Pharmaceutical Design*, **2004**, 10, 1057-67	3.3	13
38	Efficient synthesis of alpha-aryl-/heteroaryl-substituted beta-amino acids via Ni(II) complex through the Suzuki coupling reaction. *Journal of Organic Chemistry*, **2009**, 74, 5656-9	4.2	12
37	Tryptophan-containing dipeptide derivatives as potent PPARgamma antagonists: design, synthesis, biological evaluation, and molecular modeling. *European Journal of Medicinal Chemistry*, **2008**, 43, 2699-716	6.8	12
36	Steered molecular dynamics simulations on the "tail helix latch" hypothesis in the gelsolin activation process. *Biophysical Journal*, **2002**, 83, 753-62	2.9	12
35	Combinatorial Pharmacophore Modeling of Multidrug and Toxin Extrusion Transporter 1 Inhibitors: a Theoretical Perspective for Understanding Multiple Inhibitory Mechanisms. *Scientific Reports*, **2015**, 5, 13684	4.9	11
34	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. *Protein and Peptide Letters*, **2009**, 16, 150-62	1.9	11
33	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, 254-61	4	11
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31	Machine Learning-Based Modeling of Drug Toxicity. *Methods in Molecular Biology*, **2018**, 1754, 247-264	1.4	10
30	Identification of novel small molecules as inhibitors of hepatitis C virus by structure-based virtual screening. *International Journal of Molecular Sciences*, **2013**, 14, 22845-56	6.3	10
29	Dynamic mechanism of fatty acid transport across cellular membranes through FadL: molecular dynamics simulations. *Journal of Physical Chemistry B*, **2008**, 112, 13070-8	3.4	10
28	Pharmacophore-directed homology modeling and molecular dynamics simulation of G protein-coupled receptor: study of possible binding modes of 5-HT2C receptor agonists. *Acta Biochimica Et Biophysica Sinica*, **2007**, 39, 413-22	2.8	10
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25	Fragment-based prediction of skin sensitization using recursive partitioning. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 885-93	4.2	9
24	Computational models for predicting interactions with membrane transporters. *Current Medicinal Chemistry*, **2013**, 20, 2118-36	4.3	8
23	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	7.9	8
22	Drug repurposing against breast cancer by integrating drug-exposure expression profiles and drug-drug links based on graph neural network. *Bioinformatics*, **2021**,	7.2	8
21	Synthesis of polysubstituted □amino cyclohexane carboxylic acids via Diels-Alder reaction using Ni(II)-complex stabilized □alanine derived dienes. *Amino Acids*, **2013**, 44, 791-6	3.5	7
20	Deep Neural Network Classifier for Virtual Screening Inhibitors of (S)-Adenosyl-L-Methionine (SAM)-Dependent Methyltransferase Family. *Frontiers in Chemistry*, **2019**, 7, 324	5	5
19	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. *Organic and Biomolecular Chemistry*, **2006**, 4, 659-66	3.9	5
18	Steered molecular dynamics simulations of protein-ligand interactions. *Science in China Series B: Chemistry*, **2004**, 47, 355-366		4
17	Revisiting Aldehyde Oxidase Mediated Metabolism in Drug-like Molecules: An Improved Computational Model. *Journal of Medicinal Chemistry*, **2020**, 63, 6523-6537	8.3	3
16	Synthesis and biological evaluation of novel isopropanolamine derivatives as non-peptide human immunodeficiency virus protease inhibitors. *Chemical and Pharmaceutical Bulletin*, **2008**, 56, 1147-52	1.9	3
15	Hepatoprotective Effect and Potential Mechanism of Aqueous Extract from on Carbon-Tetrachloride-Induced Liver Fibrosis in Rats. *Evidence-based Complementary and Alternative Medicine*, **2021**, 2021, 5345821	2.3	3
14	Identification and evaluation of coronavirus replicase inhibitors using a replicon cell line. *Advances in Experimental Medicine and Biology*, **2006**, 581, 609-13	3.6	3
13	Diterpenoids from the Root Bark of and Evaluation of Their Phosphodiesterase Type 4D Inhibitory Activity. *Journal of Natural Products*, **2020**, 83, 1229-1237	4.9	2
12	Drug Discovery and Development: Computational Approaches **2008**, 1		2
11	Active Learning for Drug Design: A Case Study on the Plasma Exposure of Orally Administered Drugs. *Journal of Medicinal Chemistry*, **2021**, 64, 16838-16853	8.3	2
10	Computational target fishing by mining transcriptional data using a novel Siamese spectral-based graph convolutional network		2
9	Regioselective synthesis of substituted thiazoles via cascade reactions from 3-chlorochromones and thioamides. *Organic and Biomolecular Chemistry*, **2020**, 18, 6162-6170	3.9	2

8	SOMEViz: a web service for site of metabolism estimating and visualizing. *Protein and Peptide Letters*, **2012**, 19, 905-9	1.9	1
7	Computational Approaches to Drug Discovery and Development **2012**, 23-40		1
6	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	1.3	1
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3	Discovery of Cyclic Peptidomimetic Ligands Targeting the Extracellular Domain of EGFR. *Journal of Medicinal Chemistry*, **2021**, 64, 11219-11228	8.3	0
2	A hybrid framework for improving uncertainty quantification in deep learning-based QSAR regression modeling. *Journal of Cheminformatics*, **2021**, 13, 69	8.6	0
1	In Silico Prediction of Cytochrome P450-Mediated Site of Metabolism (SOM). *Protein and Peptide Letters*, **2013**, 20, 279-289	1.9	