Lei Xu

List of Publications by Year
in descending order

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42 papers	3,054 citations	471509 17 h-index	265206 42 g-index
43 all docs	43 docs citations	43 times ranked	3286 citing authors

#	Article	IF	Citations
1	Comprehensive evaluation of ten docking programs on a diverse set of proteinâ€“ligand complexes: the prediction accuracy of sampling power and scoring power. Physical Chemistry Chemical Physics, 2016, 18, 12964-12975.	2.8	669
2	Assessing the performance of MM/PBSA and MM/GBSA methods. 4. Accuracies of MM/PBSA and MM/GBSA methodologies evaluated by various simulation protocols using PDBbind data set. Physical Chemistry Chemical Physics, 2014, 16, 16719-16729.	2.8	586
3	Assessing the performance of MM/PBSA and MM/GBSA methods. 5. Improved docking performance using high solute dielectric constant MM/GBSA and MM/PBSA rescoring. Physical Chemistry Chemical Physics, 2014, 16, 22035-22045.	2.8	432
4	Assessing the Performance of MM/PBSA and MM/GBSA Methods. 3. The Impact of Force Fields and Ligand Charge Models. Journal of Physical Chemistry B, 2013, 117, 8408-8421.	2.6	419
5	The application of in silico drug-likeness predictions in pharmaceutical research. Advanced Drug Delivery Reviews, 2015, 86, 2-10.	13.7	306
6	Discovery of Novel Inhibitors Targeting the Macrophage Migration Inhibitory Factor via Structure-Based Virtual Screening and Bioassays. Journal of Medicinal Chemistry, 2014, 57, 3737-3745.	6.4	66
7	Constructing and Validating High-Performance MIEC-SVM Models in Virtual Screening for Kinases: A Better Way for Actives Discovery. Scientific Reports, 2016, 6, 24817.	3.3	59
8	Structural basis of the interactions between CXCR4 and CXCL12/SDF-1 revealed by theoretical approaches. Molecular BioSystems, 2013, 9, 2107.	2.9	39
9	Voltage-gated sodium channels: structures, functions, and molecular modeling. Drug Discovery Today, 2019, 24, 1389-1397.	6.4	36
10	Discovery of Novel Androgen Receptor Ligands by Structure-based Virtual Screening and Bioassays. Genomics, Proteomics and Bioinformatics, 2018, 16, 416-427.	6.9	32
11	Understanding microscopic binding of macrophage migration inhibitory factor with phenolic hydrazones by molecular docking, molecular dynamics simulations and free energy calculations. Molecular BioSystems, 2012, 8, 2260.	2.9	29
12	Improvement of Prediction Performance With Conjoint Molecular Fingerprint in Deep Learning. Frontiers in Pharmacology, 2020, 11, 606668.	3.5	29
13	Theoretical Studies on the Selectivity Mechanisms of Glycogen Synthase Kinase 3Î² (GSK3Î²) with Pyrazine ATP-competitive Inhibitors by 3DQSAR, Molecular Docking, Molecular Dynamics Simulation and Free Energy Calculations. Current Computer-Aided Drug Design, 2020, 16, 17-30.	1.2	24
14	Exploring the binding mechanisms of MIF to CXCR2 using theoretical approaches. Physical Chemistry Chemical Physics, 2015, 17, 3370-3382.	2.8	23
15	Integrating Machine Learning-Based Virtual Screening With Multiple Protein Structures and Bio-Assay Evaluation for Discovery of Novel GSK3Î² Inhibitors. Frontiers in Pharmacology, 2020, 11, 566058.	3.5	23
16	Theoretical studies on the selectivity mechanisms of PI3KÎ´ inhibition with marketed idelalisib and its derivatives by 3D-QSAR, molecular docking, and molecular dynamics simulation. Journal of Molecular Modeling, 2019, 25, 242.	1.8	22
17	Rational Design of Novel Phosphoinositide 3â€Kinase Gamma (PI3KÎ³) Selective Inhibitors: A Computational Investigation Integrating 3Dâ€QSAR, Molecular Docking and Molecular Dynamics Simulation. Chemistry and Biodiversity, 2019, 16, e1900105.	2.1	21
18	Insight into the selective mechanism of phosphoinositide 3â€kinase Î³ with benzothiazole and thiazolopiperidine Î³â€specific inhibitors by in silico approaches. Chemical Biology and Drug Design, 2019, 93, 818-831.	3.2	16

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19	DeepAtomicCharge: a new graph convolutional network-based architecture for accurate prediction of atomic charges. Briefings in Bioinformatics, 2021, 22, .	6.5	16
20	Discovery of a novel phosphoinositide 3-kinase gamma (PI3KÎ³) inhibitor against hematologic malignancies and theoretical studies on its PI3KÎ³-specific binding mechanisms. RSC Advances, 2019, 9, 20207-20215.	3.6	15
21	Discovery of novel selective PI3KÎ³ inhibitors through combining machine learning-based virtual screening with multiple protein structures and bio-evaluation. Journal of Advanced Research, 2022, 36, 1-13.	9.5	15
22	Discovery of novel antagonists targeting the DNA binding domain of androgen receptor by integrated docking-based virtual screening and bioassays. Acta Pharmacologica Sinica, 2022, 43, 229-239.	6.1	14
23	Unraveling the conformational determinants of LARP7 and 7SK small nuclear RNA by theoretical approaches. Molecular BioSystems, 2016, 12, 2613-2621.	2.9	13
24	Theoretical studies on the selective mechanisms of <scp>GSK</scp>3Î² and <scp>CDK</scp>2 by molecular dynamics simulations and free energy calculations. Chemical Biology and Drug Design, 2017, 89, 846-855.	3.2	13
25	Discovery of novel natural compound inhibitors targeting estrogen receptor Î± by an integrated virtual screening strategy. Journal of Molecular Modeling, 2019, 25, 278.	1.8	13
26	Integrated molecular modeling techniques to reveal selective mechanisms of inhibitors to PI3KÎ´ with marketed Idelalisib. Chemical Biology and Drug Design, 2021, 97, 1158-1169.	3.2	11
27	Discovery of a novel nonsteroidal selective glucocorticoid receptor modulator by virtual screening and bioassays. Acta Pharmacologica Sinica, 2022, 43, 2429-2438.	6.1	11
28	Advances in L-Type Calcium Channel Structures, Functions and Molecular Modeling. Current Medicinal Chemistry, 2021, 28, 514-524.	2.4	10
29	Discovery of novel MIF inhibitors that attenuate microglial inflammatory activation by structures-based virtual screening and in vitro bioassays. Acta Pharmacologica Sinica, 2022, 43, 1508-1520.	6.1	10
30	A HTRF based competitive binding assay for screening specific inhibitors of HIV-1 capsid assembly targeting the C-Terminal domain of capsid. Antiviral Research, 2019, 169, 104544.	4.1	9
31	Multitask deep networks with grid featurization achieve improved scoring performance for proteinâ€“ligand binding. Chemical Biology and Drug Design, 2020, 96, 973-983.	3.2	9
32	A multi-conformational virtual screening approach based on machine learning targeting PI3KÎ³. Molecular Diversity, 2021, 25, 1271-1282.	3.9	8
33	Discovery of highly potent and selective EGFRT790M/L858R TKIs against NSCLC based on molecular dynamic simulation. European Journal of Medicinal Chemistry, 2022, 228, 113984.	5.5	8
34	Discovery of N-(4-(Benzyloxy)-phenyl)-sulfonamide Derivatives as Novel Antagonists of the Human Androgen Receptor Targeting the Activation Function 2. Journal of Medicinal Chemistry, 2022, 65, 2507-2521.	6.4	8
35	Recent Progress of Deep Learning in Drug Discovery. Current Pharmaceutical Design, 2021, 27, 2088-2096.	1.9	7
36	Theoretical study of myriocinâ€binding mechanism targeting serine palmitoyltransferase. Chemical Biology and Drug Design, 2022, 99, 373-381.	3.2	6

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37	Exploring PI3KÎ³ binding preference with Eganelisib, Duvelisib, and Idelalisib via energetic, pharmacophore and dissociation pathway analyses. Computers in Biology and Medicine, 2022, 147, 105642.	7.0	6
38	Exploring the binding mechanisms of PDE5 with chromeno[2,3-c]pyrrol-9(2H)-one by theoretical approaches. RSC Advances, 2018, 8, 30481-30490.	3.6	5
39	Discovery of potential inhibitors targeting the kinase domain of polynucleotide kinase/phosphatase (PNKP): Homology modeling, virtual screening based on multiple conformations, and molecular dynamics simulation. Computational Biology and Chemistry, 2021, 94, 107517.	2.3	5
40	Insight into tetrodotoxin blockade and resistance mechanisms of Na_v1.2 sodium channel by theoretical approaches. Chemical Biology and Drug Design, 2018, 92, 1445-1457.	3.2	4
41	Natural-product-library-based screening for discovery of capsid C-terminal domain targeted HIV-1 inhibitors. International Journal of Antimicrobial Agents, 2020, 55, 105926.	2.5	4
42	Discovery of novel SecA inhibitors against â€œCandidatus Liberibacter asiaticusâ€•through virtual screening and biological evaluation. Chemical Biology and Drug Design, 2021, 98, 395-404.	3.2	3