Xiang-Qun Xie

List of Publications by Year
in descending order

113	3,674	147566	161609
papers	citations	31	54
		h-index	g-index

115	115	115	4920
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Deep Learning for Drug Design: an Artificial Intelligence Paradigm for Drug Discovery in the Big Data Era. AAPS Journal, 2018, 20, 58.	2.2	220
2	p62/SQSTM1/Sequestosome-1 is an N-recognin of the N-end rule pathway which modulates autophagosome biogenesis. Nature Communications, 2017, 8, 102.	5.8	178
3	AlzPlatform: An Alzheimer's Disease Domain-Specific Chemogenomics Knowledgebase for Polypharmacology and Target Identification Research. Journal of Chemical Information and Modeling, 2014, 54, 1050-1060.	2.5	177
4	TargetHunter: An In Silico Target Identification Tool for Predicting Therapeutic Potential of Small Organic Molecules Based on Chemogenomic Database. AAPS Journal, 2013, 15, 395-406.	2.2	171
5	Cryo-EM Structure of the Human Cannabinoid Receptor CB2-Gi Signaling Complex. Cell, 2020, 180, 645-654.e13.	13.5	167
6	SQSTM1/p62: A Potential Target for Neurodegenerative Disease. ACS Chemical Neuroscience, 2019, 10, 2094-2114.	1.7	107
7	3D structural model of the G-protein-coupled cannabinoid CB2 receptor. Proteins: Structure, Function and Bioinformatics, 2003, 53, 307-319.	1.5	105
8	GPCR Structure-Based Virtual Screening Approach for CB2 Antagonist Search. Journal of Chemical Information and Modeling, 2007, 47, 1626-1637.	2.5	103
9	Molecular Fingerprint-Based Artificial Neural Networks QSAR for Ligand Biological Activity Predictions. Molecular Pharmaceutics, 2012, 9, 2912-2923.	2.3	102
10	Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of $A\beta_{16-22}$ Dimer. Journal of Chemical Theory and Computation, 2019, 15, 1440-1452.	2.3	102
11	Modeling, Molecular Dynamics Simulation, and Mutation Validation for Structure of Cannabinoid Receptor 2 Based on Known Crystal Structures of GPCRs. Journal of Chemical Information and Modeling, 2014, 54, 2483-2499.	2.5	84
12	Exploiting PubChem for virtual screening. Expert Opinion on Drug Discovery, 2010, 5, 1205-1220.	2.5	77
13	GPU Accelerated Chemical Similarity Calculation for Compound Library Comparison. Journal of Chemical Information and Modeling, 2011, 51, 1521-1527.	2.5	67
14	Computational Fragment-Based Drug Design: Current Trends, Strategies, and Applications. AAPS Journal, 2018, 20, 59.	2.2	67
15	Data Mining a Small Molecule Drug Screening Representative Subset from NIH PubChem. Journal of Chemical Information and Modeling, 2008, 48, 465-475.	2.5	64
16	Generative chemistry: drug discovery with deep learning generative models. Journal of Molecular Modeling, 2021, 27, 71.	0.8	63
17	Structural Insight into Tetrameric hTRPV1 from Homology Modeling, Molecular Docking, Molecular Dynamics Simulation, Virtual Screening, and Bioassay Validations. Journal of Chemical Information and Modeling, 2015, 55, 572-588.	2.5	56
18	N-terminal arginylation generates a bimodal degron that modulates autophagic proteolysis. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E2716-E2724.	3.3	56

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19	Allosteric Modulation of Intact Î³-Secretase Structural Dynamics. Biophysical Journal, 2017, 113, 2634-2649.	0.2	55
20	Latest advances in novel cannabinoid CB$_2$ ligands for drug abuse and their therapeutic potential. Future Medicinal Chemistry, 2012, 4, 187-204.	1.1	51
21	Targeted inhibition of the type 2 cannabinoid receptor is a novel approach to reduce renalÂfibrosis. Kidney International, 2018, 94, 756-772.	2.6	48
22	Small-molecule inhibitors targeting INK4 protein p18INK4C enhance ex vivo expansion of haematopoietic stem cells. Nature Communications, 2015, 6, 6328.	5.8	47
23	Lead Discovery, Chemistry Optimization, and Biological Evaluation Studies of Novel Biamide Derivatives as CB$_2$ Receptor Inverse Agonists and Osteoclast Inhibitors. Journal of Medicinal Chemistry, 2012, 55, 9973-9987.	2.9	44
24	Deep Convolutional Generative Adversarial Network (dcGAN) Models for Screening and Design of Small Molecules Targeting Cannabinoid Receptors. Molecular Pharmaceutics, 2019, 16, 4451-4460.	2.3	43
25	Prediction of the Binding Affinities and Selectivity for CB1 and CB2 Ligands Using Homology Modeling, Molecular Docking, Molecular Dynamics Simulations, and MM-PBSA Binding Free Energy Calculations. ACS Chemical Neuroscience, 2020, 11, 1139-1158.	1.7	38
26	Regulation of autophagic proteolysis by the N-recognin SQSTM1/p62 of the N-end rule pathway. Autophagy, 2018, 14, 359-361.	4.3	36
27	Novel Triaryl Sulfonamide Derivatives as Selective Cannabinoid Receptor 2 Inverse Agonists and Osteoclast Inhibitors: Discovery, Optimization, and Biological Evaluation. Journal of Medicinal Chemistry, 2013, 56, 2045-2058.	2.9	35
28	Prediction of Orthosteric and Allosteric Regulations on Cannabinoid Receptors Using Supervised Machine Learning Classifiers. Molecular Pharmaceutics, 2019, 16, 2605-2615.	2.3	35
29	Computational systems pharmacology analysis of cannabidiol: a combination of chemogenomics-knowledgebase network analysis and integrated in silico modeling and simulation. Acta Pharmacologica Sinica, 2019, 40, 374-386.	2.8	34
30	NMR Structural Comparison of the Cytoplasmic Juxtamembrane Domains of G-protein-coupled CB1 and CB2 Receptors in Membrane Mimetic Dodecylphosphocholine Micelles. Journal of Biological Chemistry, 2005, 280, 3605-3612.	1.6	33
31	Allosteric Binding Site and Activation Mechanism of Class C G-Protein Coupled Receptors: Metabotropic Glutamate Receptor Family. AAPS Journal, 2015, 17, 737-753.	2.2	32
32	Cardiovascular Disease Chemogenomics Knowledgebase-guided Target Identification and Drug Synergy Mechanism Study of an Herbal Formula. Scientific Reports, 2016, 6, 33963.	1.6	32
33	LiCABEDS II. Modeling of Ligand Selectivity for G-Protein-Coupled Cannabinoid Receptors. Journal of Chemical Information and Modeling, 2013, 53, 11-26.	2.5	31
34	Structural insight into the serotonin (5-HT) receptor family by molecular docking, molecular dynamics simulation and systems pharmacology analysis. Acta Pharmacologica Sinica, 2019, 40, 1138-1156.	2.8	30
35	Computational Advances for the Development of Allosteric Modulators and Bitopic Ligands in G Protein-Coupled Receptors. AAPS Journal, 2015, 17, 1080-1095.	2.2	28
36	Virus-CKB: an integrated bioinformatics platform and analysis resource for COVID-19 research. Briefings in Bioinformatics, 2021, 22, 882-895.	3.2	28

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37	Structure–function analysis of the SHOC2–MRAS–PP1C holophosphatase complex. Nature, 2022, 609, 408-415.	13.7	28
38	Chemogenomics knowledgebased polypharmacology analyses of drug abuse related G-protein coupled receptors and their ligands. Frontiers in Pharmacology, 2014, 5, 3.	1.6	27
39	Integrated In Silico Fragment-Based Drug Design: Case Study with Allosteric Modulators on Metabotropic Glutamate Receptor 5. AAPS Journal, 2017, 19, 1235-1248.	2.2	27
40	A novel small-molecule antagonizes PRMT5-mediated KLF4 methylation for targeted therapy. EBioMedicine, 2019, 44, 98-111.	2.7	27
41	Calculate protein–ligand binding affinities with the extended linear interaction energy method: application on the Cathepsin S set in the D3R Grand Challenge 3. Journal of Computer-Aided Molecular Design, 2019, 33, 105-117.	1.3	27
42	Target-Selective Phototherapy Using a Ligand-Based Photosensitizer for Type 2 Cannabinoid Receptor. Chemistry and Biology, 2014, 21, 338-344.	6.2	26
43	Design and activity of AP endonuclease-1 inhibitors. Journal of Chemical Biology, 2015, 8, 79-93.	2.2	26
44	Difference and Influence of Inactive and Active States of Cannabinoid Receptor Subtype CB2: From Conformation to Drug Discovery. Journal of Chemical Information and Modeling, 2016, 56, 1152-1163.	2.5	26
45	PD-1-Targeted Discovery of Peptide Inhibitors by Virtual Screening, Molecular Dynamics Simulation, and Surface Plasmon Resonance. Molecules, 2019, 24, 3784.	1.7	26
46	Analysis of substance use and its outcomes by machine learning I. Childhood evaluation of liability to substance use disorder. Drug and Alcohol Dependence, 2020, 206, 107605.	1.6	26
47	Ligand Classifier of Adaptively Boosting Ensemble Decision Stumps (LiCABEDS) and Its Application on Modeling Ligand Functionality for 5HT-Subtype GPCR Families. Journal of Chemical Information and Modeling, 2011, 51, 521-531.	2.5	24
48	DAKB-GPCRs: An Integrated Computational Platform for Drug Abuse Related GPCRs. Journal of Chemical Information and Modeling, 2019, 59, 1283-1289.	2.5	23
49	Cytotoxic limonoids from Trichilia americana leaves. Phytochemistry, 2015, 118, 61-67.	1.4	22
50	Development and Testing of Druglike Screening Libraries. Journal of Chemical Information and Modeling, 2019, 59, 53-65.	2.5	22
51	MCCS: a novel recognition pattern-based method for fast track discovery of anti-SARS-CoV-2 drugs. Briefings in Bioinformatics, 2021, 22, 946-962.	3.2	21
52	Residue Preference Mapping of Ligand Fragments in the Protein Data Bank. Journal of Chemical Information and Modeling, 2011, 51, 807-815.	2.5	20
53	Multi-Functional Diarylurea Small Molecule Inhibitors of TRPV1 with Therapeutic Potential for Neuroinflammation. AAPS Journal, 2016, 18, 898-913.	2.2	20
54	The efficacy and safety of cilostazol as an alternative to aspirin in Chinese patients with aspirin intolerance after coronary stent implantation: a combined clinical study and computational system pharmacology analysis. Acta Pharmacologica Sinica, 2018, 39, 205-212.	2.8	20

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55	XRK3F2 Inhibition of p62-ZZ Domain Signaling Rescues Myeloma-Induced GFI1-Driven Epigenetic Repression of the Runx2 Gene in Pre-osteoblasts to Overcome Differentiation Suppression. Frontiers in Endocrinology, 2018, 9, 344.	1.5	20
56	Computational Systems Pharmacology-Target Mapping for Fentanyl-Laced Cocaine Overdose. ACS Chemical Neuroscience, 2019, 10, 3486-3499.	1.7	19
57	Conformational Studies on a Diastereoisomeric Pair of Tricyclic Nonclassical Cannabinoids by NMR Spectroscopy and Computer Molecular Modeling. Journal of Medicinal Chemistry, 1998, 41, 167-174.	2.9	18
58	Discovery of novel INK4C small-molecule inhibitors to promote human and murine hematopoietic stem cell ex vivo expansion. Scientific Reports, 2015, 5, 18115.	1.6	18
59	Chemogenomics knowledgebase and systems pharmacology for hallucinogen target identification—Salvinorin A as a case study. Journal of Molecular Graphics and Modelling, 2016, 70, 284-295.	1.3	18
60	Metal binding mediated conformational change of XPA protein:a potential cytotoxic mechanism of nickel in the nucleotide excision repair. Journal of Molecular Modeling, 2016, 22, 156.	0.8	18
61	Prediction of Drug–Drug Interactions Between Opioids and Overdosed Benzodiazepines Using Physiologically Based Pharmacokinetic (PBPK) Modeling and Simulation. Drugs in R and D, 2019, 19, 297-305.	1.1	17
62	Trisubstituted Sulfonamides: A New Chemotype for Development of Potent and Selective CB_2 Receptor Inverse Agonists. ACS Medicinal Chemistry Letters, 2013, 4, 387-392.	1.3	16
63	Determination of van der Waals Parameters Using a Double Exponential Potential for Nonbonded Divalent Metal Cations in TIP3P Solvent. Journal of Chemical Theory and Computation, 2021, 17, 1086-1097.	2.3	16
64	Expression, purification, and isotope labeling of cannabinoid CB2 receptor fragment, CB2180–233. Protein Expression and Purification, 2004, 38, 61-68.	0.6	15
65	Covalent allosteric modulation: An emerging strategy for GPCRs drug discovery. European Journal of Medicinal Chemistry, 2020, 206, 112690.	2.6	15
66	Insight into *Ginkgo biloba* L. Extract on the Improved Spatial Learning and Memory by Chemogenomics Knowledgebase, Molecular Docking, Molecular Dynamics Simulation, and Bioassay Validations. ACS Omega, 2020, 5, 2428-2439.	1.6	15
67	Integrated Multi-Class Classification and Prediction of GPCR Allosteric Modulators by Machine Learning Intelligence. Biomolecules, 2021, 11, 870.	1.8	15
68	Compound Acquisition and Prioritization Algorithm for Constructing Structurally Diverse Compound Libraries. ACS Combinatorial Science, 2011, 13, 223-231.	3.8	14
69	An insight into paracetamol and its metabolites using molecular docking and molecular dynamics simulation. Journal of Molecular Modeling, 2018, 24, 243.	0.8	14
70	Implementation of Diverse Synthetic and Strategic Approaches to Biologically Active Sulfamides. ChemistrySelect, 2021, 6, 430-469.	0.7	14
71	In Silico Prediction and Validation of CB2 Allosteric Binding Sites to Aid the Design of Allosteric Modulators. Molecules, 2022, 27, 453.	1.7	14
72	Molecular Mechanism and Kinetics of Amyloid-β_{42} Aggregate Formation: A Simulation Study. ACS Chemical Neuroscience, 2019, 10, 4643-4658.	1.7	13

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73	Structure-Based Design of Novel Biphenyl Amide Antagonists of Human Transient Receptor Potential Cation Channel Subfamily M Member 8 Channels with Potential Implications in the Treatment of Sensory Neuropathies. ACS Chemical Neuroscience, 2020, 11, 268-290.	1.7	13
74	Xie2-64, a novel CB2 receptor inverse agonist, reduces cocaine abuse-related behaviors in rodents. Neuropharmacology, 2020, 176, 108241.	2.0	13
75	ProSelection: A Novel Algorithm to Select Proper Protein Structure Subsets for in Silico Target Identification and Drug Discovery Research. Journal of Chemical Information and Modeling, 2017, 57, 2686-2698.	2.5	12
76	Analysis of substance use and its outcomes by machine learning: II. Derivation and prediction of the trajectory of substance use severity. Drug and Alcohol Dependence, 2020, 206, 107604.	1.6	12
77	Ligand Biological Activity Predictions Using Fingerprint-Based Artificial Neural Networks (FANN-QSAR). Methods in Molecular Biology, 2015, 1260, 149-164.	0.4	12
78	Effect of Interphase Structure on the Debonding of Polycarbonate from S-2 Glass Fibers. Journal of Adhesion, 1997, 64, 7-30.	1.8	10
79	Synergism of antihypertensives and cholinesterase inhibitors in Alzheimer's disease. Alzheimer's and Dementia: Translational Research and Clinical Interventions, 2018, 4, 542-555.	1.8	10
80	Insight of Captagon Abuse by Chemogenomics Knowledgebase-guided Systems Pharmacology Target Mapping Analyses. Scientific Reports, 2019, 9, 2268.	1.6	10
81	Effects of α-Mangostin Derivatives on the Alzheimer's Disease Model of Rats and Their Mechanism: A Combination of Experimental Study and Computational Systems Pharmacology Analysis. ACS Omega, 2020, 5, 9846-9863.	1.6	10
82	Differential performance of RoseTTAFold in antibody modeling. Briefings in Bioinformatics, 2022, 23, .	3.2	10
83	Linear and Nonlinear Support Vector Machine for the Classification of Human $5\text{-}HT_{1A}$ Ligand Functionality. Molecular Informatics, 2012, 31, 85-95.	1.4	9
84	Modeling skin sensitization potential of mechanistically hard-to-be-classified aniline and phenol compounds with quantum mechanistic properties. BMC Pharmacology & Toxicology, 2014, 15, 76.	1.0	9
85	Targeting cannabinoid receptor-2 pathway by phenylacetylamide suppresses the proliferation of human myeloma cells through mitotic dysregulation and cytoskeleton disruption. Molecular Carcinogenesis, 2015, 54, 1796-1806.	1.3	9
86	StemCellCKB: An Integrated Stem Cell-Specific Chemogenomics KnowledgeBase for Target Identification and Systems-Pharmacology Research. Journal of Chemical Information and Modeling, 2016, 56, 1995-2004.	2.5	9
87	A computational strategy for finding novel targets and therapeutic compounds for opioid dependence. PLoS ONE, 2018, 13, e0207027.	1.1	9
88	MCCS, a novel characterization method for protein–ligand complex. Briefings in Bioinformatics, 2021, 22, .	3.2	9
89	Binding Characterization of GPCRs-Modulator by Molecular Complex Characterizing System (MCCS). ACS Chemical Neuroscience, 2020, 11, 3333-3345.	1.7	8
90	Enhanced self-renewal of human long-term hematopoietic stem cells by a sulfamoyl benzoate derivative targeting p18INK4C. Blood Advances, 2021, 5, 3362-3372.	2.5	8

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91	In Silico Chemogenomics Knowledgebase and Computational System Neuropharmacology Approach for Cannabinoid Drug Research. , 2016, , 183-195.		8
92	Artificial Intelligent Deep Learning Molecular Generative Modeling of Scaffold-Focused and Cannabinoid CB2 Target-Specific Small-Molecule Sublibraries. Cells, 2022, 11, 915.	1.8	8
93	Advances in Methods to Characterize Ligand-Induced Ionic Lock and Rotamer Toggle Molecular Switch in G Protein-Coupled Receptors. Methods in Enzymology, 2013, 520, 153-174.	0.4	7
94	Introducing Virtual Oligomerization Inhibition to Identify Potent Inhibitors of AÎ² Oligomerization. Journal of Chemical Theory and Computation, 2020, 16, 3920-3935.	2.3	7
95	IsAb: a computational protocol for antibody design. Briefings in Bioinformatics, 2021, 22, .	3.2	7
96	Examining the critical roles of human CB2 receptor residues Valine 3.32 (113) and Leucine 5.41 (192) in ligand recognition and downstream signaling activities. Biochemical and Biophysical Research Communications, 2014, 452, 334-339.	1.0	6
97	Chemogenomics Systems Pharmacology Mapping of Potential Drug Targets for Treatment of Traumatic Brain Injury. Journal of Neurotrauma, 2019, 36, 565-575.	1.7	6
98	Significantly different effects of tetrahydroberberrubine enantiomers on dopamine D1/D2 receptors revealed by experimental study and integrated in silico simulation. Journal of Computer-Aided Molecular Design, 2019, 33, 447-459.	1.3	6
99	In silico design novel vibsanin B derivatives as inhibitor for heat shock protein 90 based on 3D-QSAR, molecular docking and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4313-4324.	2.0	6
100	Structural and in Vitro Functional Characterization of a Menthyl TRPM8 Antagonist Indicates Species-Dependent Regulation. ACS Medicinal Chemistry Letters, 2021, 12, 758-767.	1.3	6
101	Sequestsome-1/p62-targeted small molecules for pancreatic cancer therapy. Drug Discovery Today, 2022, 27, 362-370.	3.2	6
102	Drugâ€"Drug Interaction Between Oxycodone and Diazepam by a Combined *in Silico* Pharmacokinetic and Pharmacodynamic Modeling Approach. ACS Chemical Neuroscience, 2021, 12, 1777-1790.	1.7	5
103	Cancer genomics: opportunities for medicinal chemistry?. Future Medicinal Chemistry, 2016, 8, 357-359.	1.1	4
104	The p62-ZZ Domain Inhibitor XRK3F2 Alters Myeloma-Induced Suppression of Osteoblast Differentiation and Is Highly Cytotoxic to Myeloma Cells in Combination with Bortezomib. Blood, 2014, 124, 2083-2083.	0.6	4
105	p62-ZZ Domain Signaling Inhibition Rescues MM-Induced Epigenetic Repression at the Runx2 promoter and Allows Osteoblast Differentiation of MM Patient Pre-Osteoblasts In Vitro. Blood, 2016, 128, 4410-4410.	0.6	4
106	Pain-CKB, A Pain-Domain-Specific Chemogenomics Knowledgebase for Target Identification and Systems Pharmacology Research. Journal of Chemical Information and Modeling, 2020, 60, 4429-4435.	2.5	3
107	Binding Characterization of Agonists and Antagonists by MCCS: A Case Study from Adenosine A$_{2A}$ Receptor. ACS Chemical Neuroscience, 2021, 12, 1606-1620.	1.7	3
108	Pain Chemogenomics Knowledgebase (Pain-CKB) for Systems Pharmacology Target Mapping and Physiologically Based Pharmacokinetic Modeling Investigation of Opioid Drugâ€"Drug Interactions. ACS Chemical Neuroscience, 2020, 11, 3245-3258.	1.7	2

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109	Autophagy and Apoptosis Specific Knowledgebases-guided Systems Pharmacology Drug Research. Current Cancer Drug Targets, 2019, 19, 716-728.	0.8	2
110	How Do Modulators Affect the Orthosteric and Allosteric Binding Pockets?. ACS Chemical Neuroscience, 2022, 13, 959-977.	1.7	2
111	Synthesis of15N and13C selectively labeled anandamide. Journal of Labelled Compounds and Radiopharmaceuticals, 2002, 45, 775-784.	0.5	1
112	Cannabinoid Receptor CB2 Structure and CB2/Gi Signaling Mechanisms. FASEB Journal, 2019, 33, 493.12.	0.2	0
113	Targeting the p62-ZZ/N-End Rule Pathway in Multiple Myeloma Overcomes Proteasome Inhibitor-Resistance Via Induction of Necroptosis and Enhances the Bone Anabolic Effects of Proteasome Inhibitors. Blood, 2019, 134, 4391-4391.	0.6	0