Xiang-Qun Xie

List of Publications by Year
in descending order

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113 papers	3,674 citations	147566 31 h-index	161609 54 g-index
115 all docs	115 docs citations	115 times ranked	4920 citing authors

#	Article	IF	Citations
1	Sequestsome-1/p62-targeted small molecules for pancreatic cancer therapy. Drug Discovery Today, 2022, 27, 362-370.	3.2	6
2	In Silico Prediction and Validation of CB2 Allosteric Binding Sites to Aid the Design of Allosteric Modulators. Molecules, 2022, 27, 453.	1.7	14
3	How Do Modulators Affect the Orthosteric and Allosteric Binding Pockets?. ACS Chemical Neuroscience, 2022, 13, 959-977.	1.7	2
4	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
5	Differential performance of RoseTTAFold in antibody modeling. Briefings in Bioinformatics, 2022, 23, .	3.2	10
6	Structureâ€“function analysis of the SHOC2â€“MRASâ€“PP1C holophosphatase complex. Nature, 2022, 609, 408-415.	13.7	28
7	MCCS, a novel characterization method for proteinâ€“ligand complex. Briefings in Bioinformatics, 2021, 22, .	3.2	9
8	Virus-CKB: an integrated bioinformatics platform and analysis resource for COVID-19 research. Briefings in Bioinformatics, 2021, 22, 882-895.	3.2	28
9	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
10	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
11	Generative chemistry: drug discovery with deep learning generative models. Journal of Molecular Modeling, 2021, 27, 71.	0.8	63
12	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
13	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
14	IsAb: a computational protocol for antibody design. Briefings in Bioinformatics, 2021, 22, .	3.2	7
15	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
16	Integrated Multi-Class Classification and Prediction of GPCR Allosteric Modulators by Machine Learning Intelligence. Biomolecules, 2021, 11, 870.	1.8	15
17	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
18	Implementation of Diverse Synthetic and Strategic Approaches to Biologically Active Sulfamides. ChemistrySelect, 2021, 6, 430-469.	0.7	14

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19	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
20	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
21	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
22	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
23	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
24	Binding Characterization of GPCRs-Modulator by Molecular Complex Characterizing System (MCCS). ACS Chemical Neuroscience, 2020, 11, 3333-3345.	1.7	8
25	Covalent allosteric modulation: An emerging strategy for GPCRs drug discovery. European Journal of Medicinal Chemistry, 2020, 206, 112690.	2.6	15
26	Xie2-64, a novel CB2 receptor inverse agonist, reduces cocaine abuse-related behaviors in rodents. Neuropharmacology, 2020, 176, 108241.	2.0	13
27	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
28	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
29	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
30	Cryo-EM Structure of the Human Cannabinoid Receptor CB2-Gi Signaling Complex. Cell, 2020, 180, 645-654.e13.	13.5	167
31	Effects of Î±-Mangostin Derivatives on the Alzheimerâ€™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
32	Introducing Virtual Oligomerization Inhibition to Identify Potent Inhibitors of AÎ² Oligomerization. Journal of Chemical Theory and Computation, 2020, 16, 3920-3935.	2.3	7
33	Chemogenomics Systems Pharmacology Mapping of Potential Drug Targets for Treatment of Traumatic Brain Injury. Journal of Neurotrauma, 2019, 36, 565-575.	1.7	6
34	Computational Systems Pharmacology-Target Mapping for Fentanyl-Laced Cocaine Overdose. ACS Chemical Neuroscience, 2019, 10, 3486-3499.	1.7	19
35	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
36	PD-1-Targeted Discovery of Peptide Inhibitors by Virtual Screening, Molecular Dynamics Simulation, and Surface Plasmon Resonance. Molecules, 2019, 24, 3784.	1.7	26

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37	Molecular Mechanism and Kinetics of Amyloid-Î²₄₂ Aggregate Formation: A Simulation Study. ACS Chemical Neuroscience, 2019, 10, 4643-4658.	1.7	13
38	Prediction of Drugâ€“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
39	SQSTM1/p62: A Potential Target for Neurodegenerative Disease. ACS Chemical Neuroscience, 2019, 10, 2094-2114.	1.7	107
40	A novel small-molecule antagonizes PRMT5-mediated KLF4 methylation for targeted therapy. EBioMedicine, 2019, 44, 98-111.	2.7	27
41	Prediction of Orthosteric and Allosteric Regulations on Cannabinoid Receptors Using Supervised Machine Learning Classifiers. Molecular Pharmaceutics, 2019, 16, 2605-2615.	2.3	35
42	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
43	DAKB-GPCRs: An Integrated Computational Platform for Drug Abuse Related GPCRs. Journal of Chemical Information and Modeling, 2019, 59, 1283-1289.	2.5	23
44	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
45	Insight of Captagon Abuse by Chemogenomics Knowledgebase-guided Systems Pharmacology Target Mapping Analyses. Scientific Reports, 2019, 9, 2268.	1.6	10
46	Calculate proteinâ€“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
47	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
48	Development and Testing of Druglike Screening Libraries. Journal of Chemical Information and Modeling, 2019, 59, 53-65.	2.5	22
49	Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of AÎ²_{16â€“22} Dimer. Journal of Chemical Theory and Computation, 2019, 15, 1440-1452.	2.3	102
50	Autophagy and Apoptosis Specific Knowledgebases-guided Systems Pharmacology Drug Research. Current Cancer Drug Targets, 2019, 19, 716-728.	0.8	2
51	Cannabinoid Receptor CB2 Structure and CB2/Gi Signaling Mechanisms. FASEB Journal, 2019, 33, 493.12.	0.2	0
52	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
53	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
54	Computational Fragment-Based Drug Design: Current Trends, Strategies, and Applications. AAPS Journal, 2018, 20, 59.	2.2	67

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55	Regulation of autophagic proteolysis by the N-recognin SQSTM1/p62 of the N-end rule pathway. Autophagy, 2018, 14, 359-361.	4.3	36
56	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
57	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
58	A computational strategy for finding novel targets and therapeutic compounds for opioid dependence. PLoS ONE, 2018, 13, e0207027.	1.1	9
59	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
60	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
61	An insight into paracetamol and its metabolites using molecular docking and molecular dynamics simulation. Journal of Molecular Modeling, 2018, 24, 243.	0.8	14
62	Targeted inhibition of the type 2 cannabinoid receptor is a novel approach to reduce renalÂfibrosis. Kidney International, 2018, 94, 756-772.	2.6	48
63	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
64	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
65	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
66	Allosteric Modulation of Intact Î³-Secretase Structural Dynamics. Biophysical Journal, 2017, 113, 2634-2649.	0.2	55
67	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
68	Chemogenomics knowledgebase and systems pharmacology for hallucinogen target identificationâ€"Salvinorin A as a case study. Journal of Molecular Graphics and Modelling, 2016, 70, 284-295.	1.3	18
69	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
70	Cardiovascular Disease Chemogenomics Knowledgebase-guided Target Identification and Drug Synergy Mechanism Study of an Herbal Formula. Scientific Reports, 2016, 6, 33963.	1.6	32
71	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
72	Cancer genomics: opportunities for medicinal chemistry?. Future Medicinal Chemistry, 2016, 8, 357-359.	1.1	4

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73	Multi-Functional Diarylurea Small Molecule Inhibitors of TRPV1 with Therapeutic Potential for Neuroinflammation. AAPS Journal, 2016, 18, 898-913.	2.2	20
74	In Silico Chemogenomics Knowledgebase and Computational System Neuropharmacology Approach for Cannabinoid Drug Research. , 2016, , 183-195.		8
75	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
76	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
77	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
78	Targeting cannabinoid receptorâ€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
79	Small-molecule inhibitors targeting INK4 protein p18INK4C enhance ex vivo expansion of haematopoietic stem cells. Nature Communications, 2015, 6, 6328.	5.8	47
80	Design and activity of AP endonuclease-1 inhibitors. Journal of Chemical Biology, 2015, 8, 79-93.	2.2	26
81	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
82	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
83	Cytotoxic limonoids from Trichilia americana leaves. Phytochemistry, 2015, 118, 61-67.	1.4	22
84	Ligand Biological Activity Predictions Using Fingerprint-Based Artificial Neural Networks (FANN-QSAR). Methods in Molecular Biology, 2015, 1260, 149-164.	0.4	12
85	Chemogenomics knowledgebased polypharmacology analyses of drug abuse related G-protein coupled receptors and their ligands. Frontiers in Pharmacology, 2014, 5, 3.	1.6	27
86	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
87	Target-Selective Phototherapy Using a Ligand-Based Photosensitizer for Type 2 Cannabinoid Receptor. Chemistry and Biology, 2014, 21, 338-344.	6.2	26
88	AlzPlatform: An Alzheimerâ€™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
89	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
90	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

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91	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
92	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
93	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
94	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
95	Trisubstituted Sulfonamides: A New Chemotype for Development of Potent and Selective CB₂ Receptor Inverse Agonists. ACS Medicinal Chemistry Letters, 2013, 4, 387-392.	1.3	16
96	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
97	Lead Discovery, Chemistry Optimization, and Biological Evaluation Studies of Novel Biamide Derivatives as CB₂ Receptor Inverse Agonists and Osteoclast Inhibitors. Journal of Medicinal Chemistry, 2012, 55, 9973-9987.	2.9	44
98	Molecular Fingerprint-Based Artificial Neural Networks QSAR for Ligand Biological Activity Predictions. Molecular Pharmaceutics, 2012, 9, 2912-2923.	2.3	102
99	Latest advances in novel cannabinoid CB₂ ligands for drug abuse and their therapeutic potential. Future Medicinal Chemistry, 2012, 4, 187-204.	1.1	51
100	Linear and Nonlinear Support Vector Machine for the Classification of Human 5â€HT_{1A} Ligand Functionality. Molecular Informatics, 2012, 31, 85-95.	1.4	9
101	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
102	Residue Preference Mapping of Ligand Fragments in the Protein Data Bank. Journal of Chemical Information and Modeling, 2011, 51, 807-815.	2.5	20
103	Compound Acquisition and Prioritization Algorithm for Constructing Structurally Diverse Compound Libraries. ACS Combinatorial Science, 2011, 13, 223-231.	3.8	14
104	GPU Accelerated Chemical Similarity Calculation for Compound Library Comparison. Journal of Chemical Information and Modeling, 2011, 51, 1521-1527.	2.5	67
105	Exploiting PubChem for virtual screening. Expert Opinion on Drug Discovery, 2010, 5, 1205-1220.	2.5	77
106	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
107	GPCR Structure-Based Virtual Screening Approach for CB2 Antagonist Search. Journal of Chemical Information and Modeling, 2007, 47, 1626-1637.	2.5	103
108	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

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109	Expression, purification, and isotope labeling of cannabinoid CB2 receptor fragment, CB2180â€“233. Protein Expression and Purification, 2004, 38, 61-68.	0.6	15
110	3D structural model of the G-protein-coupled cannabinoid CB2 receptor. Proteins: Structure, Function and Bioinformatics, 2003, 53, 307-319.	1.5	105
111	Synthesis of15N and13C selectively labeled anandamide. Journal of Labelled Compounds and Radiopharmaceuticals, 2002, 45, 775-784.	0.5	1
112	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
113	Effect of Interphase Structure on the Debonding of Polycarbonate from S-2 Glass Fibers. Journal of Adhesion, 1997, 64, 7-30.	1.8	10