Xi-Ping Huang

List of Publications by Year
in descending order

95 papers	16,491 citations	41344 49 h-index	36028 97 g-index
112 all docs	112 docs citations	112 times ranked	23509 citing authors

#	Article	IF	Citations
1	Synthon-based ligand discovery in virtual libraries of over 11 billion compounds. Nature, 2022, 601, 452-459.	27.8	153
2	Subversion of Serotonin Receptor Signaling in Osteoblasts by Kynurenine Drives Acute Myeloid Leukemia. Cancer Discovery, 2022, 12, 1106-1127.	9.4	12
3	Structural optimizations and bioevaluation of N-H aporphine analogues as Gq-biased and selective serotonin 5-HT2C receptor agonists. Bioorganic Chemistry, 2022, 123, 105795.	4.1	2
4	Structural insights into the human D1 and D2 dopamine receptor signaling complexes. Cell, 2021, 184, 931-942.e18.	28.9	140
5	Mechanism of dopamine binding and allosteric modulation of the human D1 dopamine receptor. Cell Research, 2021, 31, 593-596.	12.0	48
6	Structures of the human dopamine D3 receptor-Gi complexes. Molecular Cell, 2021, 81, 1147-1159.e4.	9.7	51
7	COVID-19: Famotidine, Histamine, Mast Cells, and Mechanisms. Frontiers in Pharmacology, 2021, 12, 633680.	3.5	64
8	Allostery of atypical modulators at oligomeric G protein-coupled receptors. Scientific Reports, 2021, 11, 9265.	3.3	2
9	Structure, function and pharmacology of human itch GPCRs. Nature, 2021, 600, 170-175.	27.8	101
10	Structures of the Ïƒ2 receptor enable docking for bioactive ligand discovery. Nature, 2021, 600, 759-764.	27.8	113
11	The activities of drug inactive ingredients on biological targets. Science, 2020, 369, 403-413.	12.6	61
12	Differential Roles of Extracellular Histidine Residues of GPR68 for Proton-Sensing and Allosteric Modulation by Divalent Metal Ions. Biochemistry, 2020, 59, 3594-3614.	2.5	11
13	Virtual discovery of melatonin receptor ligands to modulate circadian rhythms. Nature, 2020, 579, 609-614.	27.8	184
14	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. Nature, 2020, 583, 459-468.	27.8	3,542
15	Deschloroclozapine, a potent and selective chemogenetic actuator enables rapid neuronal and behavioral modulations in mice and monkeys. Nature Neuroscience, 2020, 23, 1157-1167.	14.8	187
16	A Novel G Protein-Biased and Subtype-Selective Agonist for a G Protein-Coupled Receptor Discovered from Screening Herbal Extracts. ACS Central Science, 2020, 6, 213-225.	11.3	25
17	Design and Synthesis of Bitopic 2-Phenylcyclopropylmethylamine (PCPMA) Derivatives as Selective Dopamine D3 Receptor Ligands. Journal of Medicinal Chemistry, 2020, 63, 4579-4602.	6.4	15
18	Structure-based discovery of potent and selective melatonin receptor agonists. ELife, 2020, 9, .	6.0	28

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19	Designing Functionally Selective Noncatechol Dopamine D₁ Receptor Agonists with Potent In Vivo Antiparkinsonian Activity. ACS Chemical Neuroscience, 2019, 10, 4160-4182.	3.5	21
20	Î²-Fluorofentanyls Are pH-Sensitive Mu Opioid Receptor Agonists. ACS Medicinal Chemistry Letters, 2019, 10, 1353-1356.	2.8	18
21	Design, Synthesis, and Characterization of Ogerin-Based Positive Allosteric Modulators for G Protein-Coupled Receptor 68 (GPR68). Journal of Medicinal Chemistry, 2019, 62, 7557-7574.	6.4	16
22	Discovery of Human Signaling Systems: Pairing Peptides to G Protein-Coupled Receptors. Cell, 2019, 179, 895-908.e21.	28.9	157
23	Structural basis of ligand recognition at the human MT1 melatonin receptor. Nature, 2019, 569, 284-288.	27.8	140
24	XFEL structures of the human MT2 melatonin receptor reveal the basis of subtype selectivity. Nature, 2019, 569, 289-292.	27.8	106
25	Defining Structureâ€“Functional Selectivity Relationships (SFSR) for a Class of Non-Catechol Dopamine D₁ Receptor Agonists. Journal of Medicinal Chemistry, 2019, 62, 3753-3772.	6.4	15
26	Dezocine Alleviates Morphine-Induced Dependence in Rats. Anesthesia and Analgesia, 2019, 128, 1328-1335.	2.2	24
27	5-HT2C Receptor Structures Reveal the Structural Basis of GPCR Polypharmacology. Cell, 2018, 172, 719-730.e14.	28.9	185
28	Structure of the Nanobody-Stabilized Active State of the Kappa Opioid Receptor. Cell, 2018, 172, 55-67.e15.	28.9	299
29	Exploring Halogen Bonds in 5-Hydroxytryptamine 2B Receptorâ€“Ligand Interactions. ACS Medicinal Chemistry Letters, 2018, 9, 1019-1024.	2.8	17
30	Selectivity Challenges in Docking Screens for GPCR Targets and Antitargets. Journal of Medicinal Chemistry, 2018, 61, 6830-6845.	6.4	31
31	Protamine is an antagonist of apelin receptor, and its activity is reversed by heparin. FASEB Journal, 2017, 31, 2507-2519.	0.5	26
32	Zanos et al. reply. Nature, 2017, 546, E4-E5.	27.8	29
33	Structure-Based Discovery of New Antagonist and Biased Agonist Chemotypes for the Kappa Opioid Receptor. Journal of Medicinal Chemistry, 2017, 60, 3070-3081.	6.4	42
34	In silico design of novel probes for the atypical opioid receptor MRGPRX2. Nature Chemical Biology, 2017, 13, 529-536.	8.0	230
35	D ₄ dopamine receptor high-resolution structures enable the discovery of selective agonists. Science, 2017, 358, 381-386.	12.6	176
36	A Simple Representation of Three-Dimensional Molecular Structure. Journal of Medicinal Chemistry, 2017, 60, 7393-7409.	6.4	72

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37	Fentanyl-related designer drugs W-18 and W-15 lack appreciable opioid activity in vitro and in vivo. JCI Insight, 2017, 2, .	5.0	14
38	In Vitro and In Vivo Characterization of the Alkaloid Nuciferine. PLoS ONE, 2016, 11, e0150602.	2.5	28
39	Design and synthesis of dual 5-HT1A and 5-HT7 receptor ligands. Bioorganic and Medicinal Chemistry, 2016, 24, 3464-3471.	3.0	19
40	NMDAR inhibition-independent antidepressant actions of ketamine metabolites. Nature, 2016, 533, 481-486.	27.8	1,246
41	Effects of Ketamine and Ketamine Metabolites on Evoked Striatal Dopamine Release, Dopamine Receptors, and Monoamine Transporters. Journal of Pharmacology and Experimental Therapeutics, 2016, 359, 159-170.	2.5	89
42	Structure-based discovery of opioid analgesics with reduced side effects. Nature, 2016, 537, 185-190.	27.8	744
43	Discovery and Characterization of Novel GPR39 Agonists Allosterically Modulated by Zinc. Molecular Pharmacology, 2016, 90, 726-737.	2.3	48
44	Ïƒ1 receptor ligands control a switch between passive and active threat responses. Nature Chemical Biology, 2016, 12, 552-558.	8.0	37
45	Zebrafish behavioral profiling identifies multitarget antipsychotic-like compounds. Nature Chemical Biology, 2016, 12, 559-566.	8.0	124
46	Development of CNS multi-receptor ligands: Modification of known D2 pharmacophores. Bioorganic and Medicinal Chemistry, 2016, 24, 3671-3679.	3.0	3
47	hERG Blockade by Iboga Alkaloids. Cardiovascular Toxicology, 2016, 16, 14-22.	2.7	23
48	A cellular chemical probe targeting the chromodomains of Polycomb repressive complex 1. Nature Chemical Biology, 2016, 12, 180-187.	8.0	133
49	Further Advances in Optimizing (2-Phenylcyclopropyl)methylamines as Novel Serotonin 2C Agonists: Effects on Hyperlocomotion, Prepulse Inhibition, and Cognition Models. Journal of Medicinal Chemistry, 2016, 59, 578-591.	6.4	26
50	Structure-Based Discovery of Novel and Selective 5-Hydroxytryptamine 2B Receptor Antagonists for the Treatment of Irritable Bowel Syndrome. Journal of Medicinal Chemistry, 2016, 59, 707-720.	6.4	35
51	Comprehensive characterization of the Published Kinase Inhibitor Set. Nature Biotechnology, 2016, 34, 95-103.	17.5	289
52	The First Structureâ€“Activity Relationship Studies for Designer Receptors Exclusively Activated by Designer Drugs. ACS Chemical Neuroscience, 2015, 6, 476-484.	3.5	128
53	A New DREADD Facilitates the Multiplexed Chemogenetic Interrogation of Behavior. Neuron, 2015, 86, 936-946.	8.1	320
54	PRESTO-Tango as an open-source resource for interrogation of the druggable human GPCRome. Nature Structural and Molecular Biology, 2015, 22, 362-369.	8.2	535

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55	Selectivity and Anti-Parkinsonâ€™s Potential of Thiadiazolidinone RGS4 Inhibitors. ACS Chemical Neuroscience, 2015, 6, 911-919.	3.5	41
56	Allosteric ligands for the pharmacologically dark receptors GPR68 and GPR65. Nature, 2015, 527, 477-483.	27.8	214
57	Molecular interactions between general anesthetics and the 5HT_{2B}receptor. Journal of Biomolecular Structure and Dynamics, 2015, 33, 211-218.	3.5	10
58	Synthesis, Pharmacological Characterization, and Structureâ€“Activity Relationship Studies of Small Molecular Agonists for the Orphan GPR88 Receptor. ACS Chemical Neuroscience, 2014, 5, 576-587.	3.5	41
59	Molecular control of Î´-opioid receptor signalling. Nature, 2014, 506, 191-196.	27.8	432
60	Structural basis for Smoothened receptor modulation and chemoresistance to anticancer drugs. Nature Communications, 2014, 5, 4355.	12.8	208
61	Novel Molecular Targets of Dezocine and Their Clinical Implications. Anesthesiology, 2014, 120, 714-723.	2.5	77
62	Discovery of Î²2 Adrenergic Receptor Ligands Using Biosensor Fragment Screening of Tagged Wild-Type Receptor. ACS Medicinal Chemistry Letters, 2013, 4, 1005-1010.	2.8	65
63	Aryl Biphenylâ€3â€ylmethylpiperazines as 5â€HT₇ Receptor Antagonists. ChemMedChem, 2013, 8, 1855-1864.	3.2	12
64	Neurochemical profiles of some novel psychoactive substances. European Journal of Pharmacology, 2013, 700, 147-151.	3.5	150
65	Photochemical activation of TRPA1 channels in neurons and animals. Nature Chemical Biology, 2013, 9, 257-263.	8.0	97
66	Structural Features for Functional Selectivity at Serotonin Receptors. Science, 2013, 340, 615-619.	12.6	600
67	Structural Basis for Molecular Recognition at Serotonin Receptors. Science, 2013, 340, 610-614.	12.6	454
68	An analysis of the synthetic tryptamines AMT and 5-MeO-DALT: Emerging â€˜Novel Psychoactive Drugsâ€™. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 3411-3415.	2.2	36
69	Structure of the human smoothened receptor bound to an antitumour agent. Nature, 2013, 497, 338-343.	27.8	415
70	The Ketamine Analogue Methoxetamine and 3- and 4-Methoxy Analogues of Phencyclidine Are High Affinity and Selective Ligands for the Glutamate NMDA Receptor. PLoS ONE, 2013, 8, e59334.	2.5	132
71	Selective Îº Opioid Antagonists nor-BNI, GNTI and JDTic Have Low Affinities for Non-Opioid Receptors and Transporters. PLoS ONE, 2013, 8, e70701.	2.5	27
72	Investigation of the D 1 â€Ð 2 dopamine receptor heteromer reveals a complex signaling mechanism not limited to G q protein activation. FASEB Journal, 2013, 27, 881.1.	0.5	0

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73	trans-2-(2,5-Dimethoxy-4-iodophenyl)cyclopropylamine and trans-2-(2,5-dimethoxy-4-bromophenyl)cyclopropylamine as potent agonists for the 5-HT₂ receptor family. Beilstein Journal of Organic Chemistry, 2012, 8, 1705-1709.	2.2	14
74	Automated design of ligands to polypharmacological profiles. Nature, 2012, 492, 215-220.	27.8	698
75	Marine Algal Toxin Azaspiracid Is an Open-State Blocker of hERG Potassium Channels. Chemical Research in Toxicology, 2012, 25, 1975-1984.	3.3	72
76	Heterotropic Cooperativity within and between Protomers of an Oligomeric M₂ Muscarinic Receptor. Biochemistry, 2012, 51, 4518-4540.	2.5	8
77	Structure of the nociceptin/orphanin FQ receptor in complex with a peptide mimetic. Nature, 2012, 485, 395-399.	27.8	430
78	Structure of the human Î¹-opioid receptor in complex with JDTic. Nature, 2012, 485, 327-332.	27.8	797
79	Life Beyond Kinases: Structure-Based Discovery of Sorafenib as Nanomolar Antagonist of 5-HT Receptors. Journal of Medicinal Chemistry, 2012, 55, 5749-5759.	6.4	68
80	The Presynaptic Component of the Serotonergic System is Required for Clozapine's Efficacy. Neuropsychopharmacology, 2011, 36, 638-651.	5.4	63
81	Rational Drug Design Leading to the Identification of a Potent 5-HT_{2C} Agonist Lacking 5-HT_{2B} Activity. ACS Medicinal Chemistry Letters, 2011, 2, 929-932.	2.8	15
82	Discovery of Î²-Arrestinâ€“Biased Dopamine D ₂ Ligands for Probing Signal Transduction Pathways Essential for Antipsychotic Efficacy. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 18488-18493.	7.1	312
83	Chemical Modifications on 4-Arylpiperazine-Ethyl Carboxamide Derivatives Differentially Modulate Affinity for 5-HT1A, D4.2, and Î±2A Receptors: Synthesis and In Vitro Radioligand Binding Studies. Australian Journal of Chemistry, 2010, 63, 56.	0.9	10
84	N-Tetrahydrothiochromenoisoxazole-1-carboxamides as selective antagonists of cloned human 5-HT2B. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 5488-5490.	2.2	8
85	Identification of HumanEther-Ã-go-goRelated Gene Modulators by Three Screening Platforms in an Academic Drug-Discovery Setting. Assay and Drug Development Technologies, 2010, 8, 727-742.	1.2	67
86	Development, Validation, and Use of Quantitative Structureâ^'Activity Relationship Models of 5-Hydroxytryptamine (2B) Receptor Ligands to Identify Novel Receptor Binders and Putative Valvulopathic Compounds among Common Drugs. Journal of Medicinal Chemistry, 2010, 53, 7573-7586.	6.4	38
87	Parallel Functional Activity Profiling Reveals Valvulopathogens Are Potent 5-Hydroxytryptamine_{2B}Receptor Agonists: Implications for Drug Safety Assessment. Molecular Pharmacology, 2009, 76, 710-722.	2.3	125
88	Amisulpride is a potent 5-HT7 antagonist: relevance for antidepressant actions in vivo. Psychopharmacology, 2009, 205, 119-128.	3.1	240
89	Novel Inhibitors of Human Histone Deacetylase (HDAC) Identified by QSAR Modeling of Known Inhibitors, Virtual Screening, and Experimental Validation. Journal of Chemical Information and Modeling, 2009, 49, 461-476.	5.4	99
90	Mutational Disruption of a Conserved Disulfide Bond in Muscarinic Acetylcholine Receptors Attenuates Positive Homotropic Cooperativity between Multiple Allosteric Sites and Has Subtype-Dependent Effects on the Affinities of Muscarinic Allosteric Ligands. Molecular Pharmacology, 2007, 71, 759-768.	2.3	14

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91	Critical Amino Acid Residues of the Common Allosteric Site on the M2 Muscarinic Acetylcholine Receptor: More Similarities than Differences between the Structurally Divergent Agents Gallamine and Bis(ammonio)alkane-Type Hexamethylene-bis-[dimethyl-(3-phthalimidopropyl)ammonium]dibromide. Molecular Pharmacology, 2005, 68, 769-778.	2.3	57
92	Design, Synthesis, and Biological Characterization of Bivalent 1-Methyl-1,2,5,6-tetrahydropyridyl-1,2,5-thiadiazole Derivatives as Selective Muscarinic Agonists. Journal of Medicinal Chemistry, 2001, 44, 4563-4576.	6.4	47
93	Design and development of selective muscarinic agonists for the treatment of Alzheimer's disease: characterization of tetrahydropyrimidine derivatives and development of new approaches for improved affinity and selectivity for M1 receptors. Pharmaceutica Acta Helvetiae, 2000, 74, 135-140.	1.2	19
94	Design and development of selective muscarinic agonists for the treatment of alzheimer's disease: characterization of tetrahydropyrimidine derivatives and dev. Pharmacochemistry Library, 2000, , 135-140.	0.1	0
95	Roles of threonineâ€ƒ192 and asparagineâ€ƒ382 in agonist and antagonist interactions with M1 muscarinic receptors. British Journal of Pharmacology, 1999, 126, 735-745.	5.4	42