Xi-Ping Huang

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

101 papers	11,543 citations	43 h-index	107 g-index
112 ext. papers	14,449 ext. citations	17.5 avg, IF	5.72 L-index

#	Paper	IF	Citations
101	Structural optimizations and bioevaluation of N-H aporphine analogues as G-biased and selective serotonin 5-HT receptor agonists.. *Bioorganic Chemistry*, **2022**, 123, 105795	5.1	0
100	Synthon-based ligand discovery in virtual libraries of over 11 billion compounds.. *Nature*, **2021**,	50.4	15
99	Structures of the receptor enable docking for bioactive ligand discovery. *Nature*, **2021**,	50.4	24
98	Structure, function and pharmacology of human itch GPCRs. *Nature*, **2021**, 600, 170-175	50.4	15
97	Mechanism of dopamine binding and allosteric modulation of the human D1 dopamine receptor. *Cell Research*, **2021**, 31, 593-596	24.7	12
96	Structures of the human dopamine D3 receptor-G complexes. *Molecular Cell*, **2021**, 81, 1147-1159.e4	17.6	15
95	COVID-19: Famotidine, Histamine, Mast Cells, and Mechanisms. *Frontiers in Pharmacology*, **2021**, 12, 633680	5.6	30
94	Allostery of atypical modulators at oligomeric G protein-coupled receptors. *Scientific Reports*, **2021**, 11, 9265	4.9	1
93	Structural insights into the human D1 and D2 dopamine receptor signaling complexes. *Cell*, **2021**, 184, 931-942.e18	56.2	37
92	Virtual discovery of melatonin receptor ligands to modulate circadian rhythms. *Nature*, **2020**, 579, 609-614	50.4	88
91	A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. *Nature*, **2020**, 583, 459-468	50.4	2142
90	Deschloroclozapine, a potent and selective chemogenetic actuator enables rapid neuronal and behavioral modulations in mice and monkeys. *Nature Neuroscience*, **2020**, 23, 1157-1167	25.5	63
89	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	16.8	11
88	Design and Synthesis of Bitopic 2-Phenylcyclopropylmethylamine (PCPMA) Derivatives as Selective Dopamine D3 Receptor Ligands. *Journal of Medicinal Chemistry*, **2020**, 63, 4579-4602	8.3	5
87	COVID-19: Famotidine, Histamine, Mast Cells, and Mechanisms **2020**,		12
86	Structure-based discovery of potent and selective melatonin receptor agonists. *ELife*, **2020**, 9,	8.9	19
85	The activities of drug inactive ingredients on biological targets. *Science*, **2020**, 369, 403-413	33.3	34

84	Differential Roles of Extracellular Histidine Residues of GPR68 for Proton-Sensing and Allosteric Modulation by Divalent Metal Ions. *Biochemistry*, **2020**, 59, 3594-3614	3.2	3
83	Structural basis of ligand recognition at the human MT melatonin receptor. *Nature*, **2019**, 569, 284-288	50.4	98
82	XFEL structures of the human MT melatonin receptor reveal the basis of subtype selectivity. *Nature* , **2019**, 569, 289-292	50.4	77
81	Defining Structure-Functional Selectivity Relationships (SFSR) for a Class of Non-Catechol Dopamine D Receptor Agonists. *Journal of Medicinal Chemistry*, **2019**, 62, 3753-3772	8.3	8
80	Designing Functionally Selective Noncatechol Dopamine D Receptor Agonists with Potent In Vivo Antiparkinsonian Activity. *ACS Chemical Neuroscience*, **2019**, 10, 4160-4182	5.7	11
79	Fluorofentanyls Are pH-Sensitive Mu Opioid Receptor Agonists. *ACS Medicinal Chemistry Letters*, **2019**, 10, 1353-1356	4.3	13
78	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	8.3	5
77	Discovery of Human Signaling Systems: Pairing Peptides to G Protein-Coupled Receptors. *Cell*, **2019** , 179, 895-908.e21	56.2	65
76	Dezocine Alleviates Morphine-Induced Dependence in Rats. *Anesthesia and Analgesia*, **2019**, 128, 1328-1335	3.9	16
75	5-HT Receptor Structures Reveal the Structural Basis of GPCR Polypharmacology. *Cell*, **2018**, 172, 719-736.e14	36.2	123
74	Structure of the Nanobody-Stabilized Active State of the Kappa Opioid Receptor. *Cell*, **2018**, 172, 55-67.e15	36.2	205
73	Selectivity Challenges in Docking Screens for GPCR Targets and Antitargets. *Journal of Medicinal Chemistry*, **2018**, 61, 6830-6845	8.3	24
72	Exploring Halogen Bonds in 5-Hydroxytryptamine 2B Receptor-Ligand Interactions. *ACS Medicinal Chemistry Letters*, **2018**, 9, 1019-1024	4.3	13
71	Protamine is an antagonist of apelin receptor, and its activity is reversed by heparin. *FASEB Journal*, **2017**, 31, 2507-2519	0.9	17
70	Zanos et al. reply. *Nature*, **2017**, 546, E4-E5	50.4	21
69	Structure-Based Discovery of New Antagonist and Biased Agonist Chemotypes for the Kappa Opioid Receptor. *Journal of Medicinal Chemistry*, **2017**, 60, 3070-3081	8.3	35
68	In silico design of novel probes for the atypical opioid receptor MRGPRX2. *Nature Chemical Biology*, **2017**, 13, 529-536	11.7	158
67	D dopamine receptor high-resolution structures enable the discovery of selective agonists. *Science*, **2017**, 358, 381-386	33.3	128

66	A Simple Representation of Three-Dimensional Molecular Structure. *Journal of Medicinal Chemistry*, **2017**, 60, 7393-7409	8.3	45
65	Fentanyl-related designer drugs W-18 and W-15 lack appreciable opioid activity in vitro and in vivo. *JCI Insight*, **2017**, 2,	9.9	11
64	Structure-based discovery of opioid analgesics with reduced side effects. *Nature*, **2016**, 537, 185-190	50.4	547
63	Discovery and Characterization of Novel GPR39 Agonists Allosterically Modulated by Zinc. *Molecular Pharmacology*, **2016**, 90, 726-737	4.3	26
62	1 receptor ligands control a switch between passive and active threat responses. *Nature Chemical Biology*, **2016**, 12, 552-8	11.7	29
61	Zebrafish behavioral profiling identifies multitarget antipsychotic-like compounds. *Nature Chemical Biology*, **2016**, 12, 559-66	11.7	81
60	Development of CNS multi-receptor ligands: Modification of known D2 pharmacophores. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 3671-9	3.4	3
59	hERG Blockade by Iboga Alkaloids. *Cardiovascular Toxicology*, **2016**, 16, 14-22	3.4	18
58	A cellular chemical probe targeting the chromodomains of Polycomb repressive complex 1. *Nature Chemical Biology*, **2016**, 12, 180-7	11.7	100
57	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, 578-91	8.3	20
56	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, 707-20	8.3	25
55	Comprehensive characterization of the Published Kinase Inhibitor Set. *Nature Biotechnology*, **2016**, 34, 95-103	44.5	191
54	In Vitro and In Vivo Characterization of the Alkaloid Nuciferine. *PLoS ONE*, **2016**, 11, e0150602	3.7	18
53	Design and synthesis of dual 5-HT1A and 5-HT7 receptor ligands. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 3464-71	3.4	16
52	NMDAR inhibition-independent antidepressant actions of ketamine metabolites. *Nature*, **2016**, 533, 481-6	50.4	903
51	Effects of Ketamine and Ketamine Metabolites on Evoked Striatal Dopamine Release, Dopamine Receptors, and Monoamine Transporters. *Journal of Pharmacology and Experimental Therapeutics*, **2016**, 359, 159-70	4.7	61
50	The first structure-activity relationship studies for designer receptors exclusively activated by designer drugs. *ACS Chemical Neuroscience*, **2015**, 6, 476-84	5.7	99
49	A New DREADD Facilitates the Multiplexed Chemogenetic Interrogation of Behavior. *Neuron*, **2015**, 86, 936-946	13.9	239

48	PRESTO-Tango as an open-source resource for interrogation of the druggable human GPCRome. *Nature Structural and Molecular Biology*, **2015**, 22, 362-9	17.6	305
47	Selectivity and anti-Parkinson's potential of thiadiazolidinone RGS4 inhibitors. *ACS Chemical Neuroscience*, **2015**, 6, 911-9	5.7	34
46	Allosteric ligands for the pharmacologically dark receptors GPR68 and GPR65. *Nature*, **2015**, 527, 477-83	50.4	158
45	Molecular interactions between general anesthetics and the 5HT2B receptor. *Journal of Biomolecular Structure and Dynamics*, **2015**, 33, 211-8	3.6	8
44	A Potent, Selective and Cell-Active Allosteric Inhibitor of Protein Arginine Methyltransferase 3 (PRMT3). *Angewandte Chemie*, **2015**, 127, 5255-5259	3.6	2
43	Synthesis, pharmacological characterization, and structure-activity relationship studies of small molecular agonists for the orphan GPR88 receptor. *ACS Chemical Neuroscience*, **2014**, 5, 576-87	5.7	31
42	Molecular control of δ-opioid receptor signalling. *Nature*, **2014**, 506, 191-6	50.4	355
41	Structural basis for Smoothened receptor modulation and chemoresistance to anticancer drugs. *Nature Communications*, **2014**, 5, 4355	17.4	175
40	Novel molecular targets of dezocine and their clinical implications. *Anesthesiology*, **2014**, 120, 714-23	4.3	65
39	Discovery of β2 Adrenergic Receptor Ligands Using Biosensor Fragment Screening of Tagged Wild-Type Receptor. *ACS Medicinal Chemistry Letters*, **2013**, 4, 1005-1010	4.3	55
38	Aryl biphenyl-3-ylmethylpiperazines as 5-HT7 receptor antagonists. *ChemMedChem*, **2013**, 8, 1855-64	3.7	12
37	Neurochemical profiles of some novel psychoactive substances. *European Journal of Pharmacology*, **2013**, 700, 147-51	5.3	132
36	Photochemical activation of TRPA1 channels in neurons and animals. *Nature Chemical Biology*, **2013**, 9, 257-63	11.7	72
35	Structural features for functional selectivity at serotonin receptors. *Science*, **2013**, 340, 615-9	33.3	492
34	Structural basis for molecular recognition at serotonin receptors. *Science*, **2013**, 340, 610-4	33.3	370
33	An analysis of the synthetic tryptamines AMT and 5-MeO-DALT: emerging 'Novel Psychoactive Drugs' *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 3411-5	2.9	24
32	Structure of the human smoothened receptor bound to an antitumour agent. *Nature*, **2013**, 497, 338-43	50.4	375
31	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	3.7	114

30	Selective □opioid antagonists nor-BNI, GNTI and JDTic have low affinities for non-opioid receptors and transporters. *PLoS ONE*, **2013**, 8, e70701	3.7	21
29	Investigation of the D1-D2 dopamine receptor heteromer reveals a complex signaling mechanism not limited to Gq protein activation. *FASEB Journal*, **2013**, 27, 881.1	0.9	
28	trans-2-(2,5-Dimethoxy-4-iodophenyl)cyclopropylamine and trans-2-(2,5-dimethoxy-4-bromophenyl)cyclopropylamine as potent agonists for the 5-HT(2) receptor family. *Beilstein Journal of Organic Chemistry*, **2012**, 8, 1705-9	2.5	11
27	Automated design of ligands to polypharmacological profiles. *Nature*, **2012**, 492, 215-20	50.4	535
26	Marine algal toxin azaspiracid is an open-state blocker of hERG potassium channels. *Chemical Research in Toxicology*, **2012**, 25, 1975-84	4	64
25	Heterotropic cooperativity within and between protomers of an oligomeric M(2) muscarinic receptor. *Biochemistry*, **2012**, 51, 4518-40	3.2	7
24	Structure of the nociceptin/orphanin FQ receptor in complex with a peptide mimetic. *Nature*, **2012**, 485, 395-9	50.4	383
23	Structure of the human □opioid receptor in complex with JDTic. *Nature*, **2012**, 485, 327-32	50.4	695
22	Life beyond kinases: structure-based discovery of sorafenib as nanomolar antagonist of 5-HT receptors. *Journal of Medicinal Chemistry*, **2012**, 55, 5749-59	8.3	57
21	The presynaptic component of the serotonergic system is required for clozapine□s efficacy. *Neuropsychopharmacology*, **2011**, 36, 638-51	8.7	55
20	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	4.3	14
19	Discovery of □arrestin-biased dopamine D2 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, 18488-93	11.5	261
18	Identification of human Ether-□go-go related gene modulators by three screening platforms in an academic drug-discovery setting. *Assay and Drug Development Technologies*, **2010**, 8, 727-42	2.1	55
17	Development, validation, and use of quantitative structure-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, 7573-86	8.3	32
16	Chemical Modifications on 4-Arylpiperazine-Ethyl Carboxamide Derivatives Differentially Modulate Affinity for 5-HT1A, D4.2, and □A Receptors: Synthesis and In Vitro Radioligand Binding Studies. *Australian Journal of Chemistry*, **2010**, 63, 56	1.2	10
15	N-tetrahydrothiochromenoisoxazole-1-carboxamides as selective antagonists of cloned human 5-HT2B. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 5488-90	2.9	7
14	Parallel functional activity profiling reveals valvulopathogens are potent 5-hydroxytryptamine(2B) receptor agonists: implications for drug safety assessment. *Molecular Pharmacology*, **2009**, 76, 710-22	4.3	111
13	Amisulpride is a potent 5-HT7 antagonist: relevance for antidepressant actions in vivo. *Psychopharmacology*, **2009**, 205, 119-28	4.7	200

List of Publications

12	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, 461-76	6.1	85
11	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*	4.3	13
10	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* **2004**, 65, 764-78	4.3	53
9	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, 4563-76	8.3	42
8	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, 135-40		16
7	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		
6	Roles of threonine 192 and asparagine 382 in agonist and antagonist interactions with M1 muscarinic receptors. *British Journal of Pharmacology*, **1999**, 126, 735-45	8.6	40
5	COVID-19: Famotidine, Histamine, Mast Cells, and Mechanisms		5
4	COVID-19: Famotidine, Histamine, Mast Cells, and Mechanisms		2
3	Pharmacology of W-18 and W-15		1
2	Deschloroclozapine, a potent and selective chemogenetic actuator enables rapid neuronal and behavioral modulations in mice and monkeys		2
1	Crystal structures of the 2 receptor template large-library docking for selective chemotypes active in vivo		5