# Xi-Ping Huang

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. Nature, 2020, 583, 459-468. | 27.8 | 3,542 |
| 2 | NMDAR inhibition-independent antidepressant actions of ketamine metabolites. Nature, 2016, 533, 481-486. | 27.8 | 1,246 |
| 3 | Structure of the human Î¼-opioid receptor in complex with JDTic. Nature, 2012, 485, 327-332. | 27.8 | 797 |
| 4 | Structure-based discovery of opioid analgesics with reduced side effects. Nature, 2016, 537, 185-190. | 27.8 | 744 |
| 5 | Automated design of ligands to polypharmacological profiles. Nature, 2012, 492, 215-220. | 27.8 | 698 |
| 6 | Structural Features for Functional Selectivity at Serotonin Receptors. Science, 2013, 340, 615-619. | 12.6 | 600 |
| 7 | 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 |
| 8 | Structural Basis for Molecular Recognition at Serotonin Receptors. Science, 2013, 340, 610-614. | 12.6 | 454 |
| 9 | Molecular control of Î´-opioid receptor signalling. Nature, 2014, 506, 191-196. | 27.8 | 432 |
| 10 | Structure of the nociceptin/orphanin FQ receptor in complex with a peptide mimetic. Nature, 2012, 485, 395-399. | 27.8 | 430 |
| 11 | Structure of the human smoothened receptor bound to an antitumour agent. Nature, 2013, 497, 338-343. | 27.8 | 415 |
| 12 | A New DREADD Facilitates the Multiplexed Chemogenetic Interrogation of Behavior. Neuron, 2015, 86, 936-946. | 8.1 | 320 |
| 13 | Discovery of Î²-Arrestinâ€“Biased Dopamine D <sub>2</sub> 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 |
| 14 | Structure of the Nanobody-Stabilized Active State of the Kappa Opioid Receptor. Cell, 2018, 172, 55-67.e15. | 28.9 | 299 |
| 15 | Comprehensive characterization of the Published Kinase Inhibitor Set. Nature Biotechnology, 2016, 34, 95-103. | 17.5 | 289 |
| 16 | Amisulpride is a potent 5-HT7 antagonist: relevance for antidepressant actions in vivo. Psychopharmacology, 2009, 205, 119-128. | 3.1 | 240 |
| 17 | In silico design of novel probes for the atypical opioid receptor MRGPRX2. Nature Chemical Biology, 2017, 13, 529-536. | 8.0 | 230 |
| 18 | Allosteric ligands for the pharmacologically dark receptors GPR68 and GPR65. Nature, 2015, 527, 477-483. | 27.8 | 214 |

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|---|---|---|---|
| 19 | Structural basis for Smoothened receptor modulation and chemoresistance to anticancer drugs. Nature Communications, 2014, 5, 4355. | 12.8 | 208 |
| 20 | 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 |
| 21 | 5-HT2C Receptor Structures Reveal the Structural Basis of GPCR Polypharmacology. Cell, 2018, 172, 719-730.e14. | 28.9 | 185 |
| 22 | Virtual discovery of melatonin receptor ligands to modulate circadian rhythms. Nature, 2020, 579, 609-614. | 27.8 | 184 |
| 23 | D <sub>4</sub> dopamine receptor high-resolution structures enable the discovery of selective agonists. Science, 2017, 358, 381-386. | 12.6 | 176 |
| 24 | Discovery of Human Signaling Systems: Pairing Peptides to G Protein-Coupled Receptors. Cell, 2019, 179, 895-908.e21. | 28.9 | 157 |
| 25 | Synthon-based ligand discovery in virtual libraries of over 11 billion compounds. Nature, 2022, 601, 452-459. | 27.8 | 153 |
| 26 | Neurochemical profiles of some novel psychoactive substances. European Journal of Pharmacology, 2013, 700, 147-151. | 3.5 | 150 |
| 27 | Structural basis of ligand recognition at the human MT1 melatonin receptor. Nature, 2019, 569, 284-288. | 27.8 | 140 |
| 28 | Structural insights into the human D1 and D2 dopamine receptor signaling complexes. Cell, 2021, 184, 931-942.e18. | 28.9 | 140 |
| 29 | A cellular chemical probe targeting the chromodomains of Polycomb repressive complex 1. Nature Chemical Biology, 2016, 12, 180-187. | 8.0 | 133 |
| 30 | 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 |
| 31 | The First Structureâ€“Activity Relationship Studies for Designer Receptors Exclusively Activated by Designer Drugs. ACS Chemical Neuroscience, 2015, 6, 476-484. | 3.5 | 128 |
| 32 | Parallel Functional Activity Profiling Reveals Valvulopathogens Are Potent 5-Hydroxytryptamine<sub>2B</sub>Receptor Agonists: Implications for Drug Safety Assessment. Molecular Pharmacology, 2009, 76, 710-722. | 2.3 | 125 |
| 33 | Zebrafish behavioral profiling identifies multitarget antipsychotic-like compounds. Nature Chemical Biology, 2016, 12, 559-566. | 8.0 | 124 |
| 34 | Structures of the Ïƒ2 receptor enable docking for bioactive ligand discovery. Nature, 2021, 600, 759-764. | 27.8 | 113 |
| 35 | XFEL structures of the human MT2 melatonin receptor reveal the basis of subtype selectivity. Nature, 2019, 569, 289-292. | 27.8 | 106 |
| 36 | Structure, function and pharmacology of human itch GPCRs. Nature, 2021, 600, 170-175. | 27.8 | 101 |

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|---|---|---|---|
| 37 | 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 |
| 38 | Photochemical activation of TRPA1 channels in neurons and animals. Nature Chemical Biology, 2013, 9, 257-263. | 8.0 | 97 |
| 39 | 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 |
| 40 | Novel Molecular Targets of Dezocine and Their Clinical Implications. Anesthesiology, 2014, 120, 714-723. | 2.5 | 77 |
| 41 | Marine Algal Toxin Azaspiracid Is an Open-State Blocker of hERG Potassium Channels. Chemical Research in Toxicology, 2012, 25, 1975-1984. | 3.3 | 72 |
| 42 | A Simple Representation of Three-Dimensional Molecular Structure. Journal of Medicinal Chemistry, 2017, 60, 7393-7409. | 6.4 | 72 |
| 43 | 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 |
| 44 | 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 |
| 45 | 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 |
| 46 | COVID-19: Famotidine, Histamine, Mast Cells, and Mechanisms. Frontiers in Pharmacology, 2021, 12, 633680. | 3.5 | 64 |
| 47 | The Presynaptic Component of the Serotonergic System is Required for Clozapine's Efficacy. Neuropsychopharmacology, 2011, 36, 638-651. | 5.4 | 63 |
| 48 | The activities of drug inactive ingredients on biological targets. Science, 2020, 369, 403-413. | 12.6 | 61 |
| 49 | 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 |
| 50 | Structures of the human dopamine D3 receptor-Gi complexes. Molecular Cell, 2021, 81, 1147-1159.e4. | 9.7 | 51 |
| 51 | Discovery and Characterization of Novel GPR39 Agonists Allosterically Modulated by Zinc. Molecular Pharmacology, 2016, 90, 726-737. | 2.3 | 48 |
| 52 | Mechanism of dopamine binding and allosteric modulation of the human D1 dopamine receptor. Cell Research, 2021, 31, 593-596. | 12.0 | 48 |
| 53 | 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 |
| 54 | 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 |

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| 55 | 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 |
| 56 | 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 |
| 57 | Selectivity and Anti-Parkinsonâ€™s Potential of Thiadiazolidinone RGS4 Inhibitors. ACS Chemical Neuroscience, 2015, 6, 911-919. | 3.5 | 41 |
| 58 | 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 |
| 59 | Ïƒ1 receptor ligands control a switch between passive and active threat responses. Nature Chemical Biology, 2016, 12, 552-558. | 8.0 | 37 |
| 60 | 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 |
| 61 | 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 |
| 62 | Selectivity Challenges in Docking Screens for GPCR Targets and Antitargets. Journal of Medicinal Chemistry, 2018, 61, 6830-6845. | 6.4 | 31 |
| 63 | Zanos et al. reply. Nature, 2017, 546, E4-E5. | 27.8 | 29 |
| 64 | In Vitro and In Vivo Characterization of the Alkaloid Nuciferine. PLoS ONE, 2016, 11, e0150602. | 2.5 | 28 |
| 65 | Structure-based discovery of potent and selective melatonin receptor agonists. ELife, 2020, 9, . | 6.0 | 28 |
| 66 | 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 |
| 67 | 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 |
| 68 | Protamine is an antagonist of apelin receptor, and its activity is reversed by heparin. FASEB Journal, 2017, 31, 2507-2519. | 0.5 | 26 |
| 69 | 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 |
| 70 | Dezocine Alleviates Morphine-Induced Dependence in Rats. Anesthesia and Analgesia, 2019, 128, 1328-1335. | 2.2 | 24 |
| 71 | hERG Blockade by Iboga Alkaloids. Cardiovascular Toxicology, 2016, 16, 14-22. | 2.7 | 23 |
| 72 | Designing Functionally Selective Noncatechol Dopamine D<sub>1</sub> Receptor Agonists with Potent In Vivo Antiparkinsonian Activity. ACS Chemical Neuroscience, 2019, 10, 4160-4182. | 3.5 | 21 |

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|---|---|---|---|
| 73 | 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 |
| 74 | Design and synthesis of dual 5-HT1A and 5-HT7 receptor ligands. Bioorganic and Medicinal Chemistry, 2016, 24, 3464-3471. | 3.0 | 19 |
| 75 | Î²-Fluorofentanyls Are pH-Sensitive Mu Opioid Receptor Agonists. ACS Medicinal Chemistry Letters, 2019, 10, 1353-1356. | 2.8 | 18 |
| 76 | Exploring Halogen Bonds in 5-Hydroxytryptamine 2B Receptorâ€“Ligand Interactions. ACS Medicinal Chemistry Letters, 2018, 9, 1019-1024. | 2.8 | 17 |
| 77 | 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 |
| 78 | Rational Drug Design Leading to the Identification of a Potent 5-HT<sub>2C</sub> Agonist Lacking 5-HT<sub>2B</sub> Activity. ACS Medicinal Chemistry Letters, 2011, 2, 929-932. | 2.8 | 15 |
| 79 | Defining Structureâ€“Functional Selectivity Relationships (SFSR) for a Class of Non-Catechol Dopamine D<sub>1</sub> Receptor Agonists. Journal of Medicinal Chemistry, 2019, 62, 3753-3772. | 6.4 | 15 |
| 80 | 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 |
| 81 | 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 |
| 82 | trans-2-(2,5-Dimethoxy-4-iodophenyl)cyclopropylamine and trans-2-(2,5-dimethoxy-4-bromophenyl)cyclopropylamine as potent agonists for the 5-HT<sub>2</sub> receptor family. Beilstein Journal of Organic Chemistry, 2012, 8, 1705-1709. | 2.2 | 14 |
| 83 | 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 |
| 84 | Aryl Biphenylâ€3â€ylmethylpiperazines as 5â€HT<sub>7</sub> Receptor Antagonists. ChemMedChem, 2013, 8, 1855-1864. | 3.2 | 12 |
| 85 | Subversion of Serotonin Receptor Signaling in Osteoblasts by Kynurenine Drives Acute Myeloid Leukemia. Cancer Discovery, 2022, 12, 1106-1127. | 9.4 | 12 |
| 86 | 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 |
| 87 | 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 |
| 88 | Molecular interactions between general anesthetics and the 5HT<sub>2B</sub>receptor. Journal of Biomolecular Structure and Dynamics, 2015, 33, 211-218. | 3.5 | 10 |
| 89 | N-Tetrahydrothiochromenoisoxazole-1-carboxamides as selective antagonists of cloned human 5-HT2B. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 5488-5490. | 2.2 | 8 |
| 90 | Heterotropic Cooperativity within and between Protomers of an Oligomeric M<sub>2</sub> Muscarinic Receptor. Biochemistry, 2012, 51, 4518-4540. | 2.5 | 8 |

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| 91 | Development of CNS multi-receptor ligands: Modification of known D2 pharmacophores. Bioorganic and Medicinal Chemistry, 2016, 24, 3671-3679. | 3.0 | 3 |
| 92 | Allostery of atypical modulators at oligomeric G protein-coupled receptors. Scientific Reports, 2021, 11, 9265. | 3.3 | 2 |
| 93 | 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 |
| 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 | 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 |