JesÃºs Giraldo

List of Publications by Year
in descending order

116 papers	2,739 citations	218381 26 h-index	223531 46 g-index
122 all docs	122 docs citations	122 times ranked	3373 citing authors

#	Article	IF	Citations
1	Remote local photoactivation of morphine produces analgesia without opioidâ€related adverse effects. British Journal of Pharmacology, 2023, 180, 958-974.	2.7	15
2	Spontaneous changes in brain striatal dopamine synthesis and storage dynamics ex vivo reveal end-product feedback-inhibition of tyrosine hydroxylase. Neuropharmacology, 2022, 212, 109058.	2.0	6
3	In Silico Assessment of the Lipid Fingerprint Signature of ATP2, the Essential P4-ATPase of Malaria Parasites. Membranes, 2022, 12, 702.	1.4	1
4	Discovery of a true bivalent dopamine D2 receptor agonist. European Journal of Medicinal Chemistry, 2021, 212, 113151.	2.6	5
5	Analysis of the Function of Receptor Oligomers by Operational Models of Agonism. , 2021, , .		0
6	Structural Assessment of Agonist Efficacy in the Î¼-Opioid Receptor: Morphine and Fentanyl Elicit Different Activation Patterns. Journal of Chemical Information and Modeling, 2021, 61, 1251-1274.	2.5	31
7	Dynamical Correlations Reveal Allosteric Sites in G Protein-Coupled Receptors. International Journal of Molecular Sciences, 2021, 22, 187.	1.8	6
8	Evaluation of Operational Models of Agonism and Allosterism at Receptors with Multiple Orthosteric Binding Sites. Molecular Pharmacology, 2020, 97, 35-45.	1.0	17
9	Statistics for the analysis of molecular dynamics simulations: providing P values for agonist-dependent GPCR activation. Scientific Reports, 2020, 10, 19942.	1.6	6
10	Exploring the Activation Mechanism of the mGlu5 Transmembrane Domain. Frontiers in Molecular Biosciences, 2020, 7, 38.	1.6	4
11	Insights into adenosine A2AÂreceptor activation through cooperative modulation of agonist and allosteric lipid interactions. PLoS Computational Biology, 2020, 16, e1007818.	1.5	20
12	Title is missing!. , 2020, 16, e1007818.		0
13	Title is missing!. , 2020, 16, e1007818.		0
14	Title is missing!. , 2020, 16, e1007818.		0
15	Title is missing!. , 2020, 16, e1007818.		0
16	Artificial Intelligence: A Novel Approach for Drug Discovery. Trends in Pharmacological Sciences, 2019, 40, 550-551.	4.0	38
17	Can Adding Constitutive Receptor Activity Redefine Biased Signaling Quantification?. Trends in Pharmacological Sciences, 2019, 40, 156-160.	4.0	11
18	Revealing the Mechanism of Agonist-Mediated Cannabinoid Receptor 1 (CB1) Activation and Phospholipid-Mediated Allosteric Modulation. Journal of Medicinal Chemistry, 2019, 62, 5638-5654.	2.9	16

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19	Distinct Dopamine D2 Receptor Antagonists Differentially Impact D2 Receptor Oligomerization. International Journal of Molecular Sciences, 2019, 20, 1686.	1.8	27
20	A method for the quantification of biased signalling at constitutively active receptors. British Journal of Pharmacology, 2018, 175, 2046-2062.	2.7	20
21	Systematic Analysis of Primary Sequence Domain Segments for the Discrimination Between Class C GPCR Subtypes. Interdisciplinary Sciences, Computational Life Sciences, 2018, 10, 43-52.	2.2	7
22	An operational model for GPCR homodimers and its application in the analysis of biased signaling. Drug Discovery Today, 2018, 23, 1591-1595.	3.2	14
23	Structural insights into positive and negative allosteric regulation of a G protein-coupled receptor through protein-lipid interactions. Scientific Reports, 2018, 8, 4456.	1.6	35
24	Dynamic modulation of inflammatory pain-related affective and sensory symptoms by optical control of amygdala metabotropic glutamate receptor 4. Molecular Psychiatry, 2018, 23, 509-520.	4.1	56
25	Quantifying the allosteric interactions within a G-protein-coupled receptor heterodimer. Drug Discovery Today, 2018, 23, 7-11.	3.2	2
26	Synthesis toward Bivalent Ligands for the Dopamine D₂ and Metabotropic Glutamate 5 Receptors. Journal of Medicinal Chemistry, 2018, 61, 8212-8225.	2.9	21
27	Using machine learning tools for protein database biocuration assistance. Scientific Reports, 2018, 8, 10148.	1.6	5
28	Representation Learning for Class C G Protein-Coupled Receptors Classification. Molecules, 2018, 23, 690.	1.7	3
29	Positional isomers of bispyridine benzene derivatives induce efficacy changes on mGlu5 negative allosteric modulation. European Journal of Medicinal Chemistry, 2017, 127, 567-576.	2.6	14
30	120. Patterns of Response to Fear learning: A Data-Driven Approach to a Biomarker of Generalized Anxiety Disorders. Biological Psychiatry, 2017, 81, S50-S51.	0.7	0
31	Illuminating Phenylazopyridines To Photoswitch Metabotropic Glutamate Receptors: From the Flask to the Animals. ACS Central Science, 2017, 3, 81-91.	5.3	58
32	Angiotensin II type 1/adenosine A 2A receptor oligomers: a novel target for tardive dyskinesia. Scientific Reports, 2017, 7, 1857.	1.6	11
33	Analysis of positive and negative allosteric modulation in metabotropic glutamate receptors 4 and 5 with a dual ligand. Scientific Reports, 2017, 7, 4944.	1.6	14
34	Text mining and expert curation to develop a database on psychiatric diseases and their genes. Database: the Journal of Biological Databases and Curation, 2017, 2017, .	1.4	11
35	A Complementary Scale of Biased Agonism for Agonists with Differing Maximal Responses. Scientific Reports, 2017, 7, 15389.	1.6	24
36	Optical control of pain in vivo with a photoactive mGlu5 receptor negative allosteric modulator. ELife, 2017, 6, .	2.8	48

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37	Pharmacological evidence for a metabotropic glutamate receptor heterodimer in neuronal cells. ELife, 2017, 6, .	2.8	63
38	Allosteric control of an asymmetric transduction in a G protein-coupled receptor heterodimer. ELife, 2017, 6, .	2.8	48
39	Have many estimates of efficacy and affinity been misled? Revisiting the operational model of agonism. Drug Discovery Today, 2016, 21, 1735-1739.	3.2	7
40	OptoGluNAM4.1, a Photoswitchable Allosteric Antagonist for Real-Time Control of mGlu 4 Receptor Activity. Cell Chemical Biology, 2016, 23, 929-934.	2.5	68
41	GNAO1 encephalopathy: further delineation of a severe neurodevelopmental syndrome affecting females. Orphanet Journal of Rare Diseases, 2016, 11, 38.	1.2	36
42	Paternal Age and Numerical Chromosome Abnormalities in Human Spermatozoa. Cytogenetic and Genome Research, 2016, 148, 241-248.	0.6	18
43	Persistence of Breakage in Specific Chromosome Bands 6 Years after Acute Exposure to Oil. PLoS ONE, 2016, 11, e0159404.	1.1	8
44	Shining Light on an mGlu5 Photoswitchable NAM: A Theoretical Perspective. Current Neuropharmacology, 2016, 14, 441-454.	1.4	18
45	Visual Exploratory Assessment of Class C GPCR Extracellular Domains Discrimination Capabilities. Advances in Intelligent Systems and Computing, 2016, , 31-39.	0.5	0
46	Label noise in subtype discrimination of class C G protein-coupled receptors: A systematic approach to the analysis of classification errors. BMC Bioinformatics, 2015, 16, 314.	1.2	8
47	Human Genotoxic Study Carried Out Two Years after Oil Exposure during the Clean-up Activities Using Two Different Biomarkers. Journal of Marine Science and Engineering, 2015, 3, 1334-1348.	1.2	3
48	Rational design of a peptide capture agent for CXCL8 based on a model of the CXCL8:CXCR1 complex. RSC Advances, 2015, 5, 25657-25668.	1.7	14
49	Quantifying conformational changes in GPCRs: glimpse of a common functional mechanism. BMC Bioinformatics, 2015, 16, 124.	1.2	45
50	The extracellular N-terminal domain suffices to discriminate class C G Protein-Coupled Receptor subtypes from n-grams of their sequences. , 2015, , .		3
51	Terminating evolutionary algorithms at their steady state. Computational Optimization and Applications, 2015, 61, 489-515.	0.9	2
52	Operational models of allosteric modulation: caution is needed. Trends in Pharmacological Sciences, 2015, 36, 1-2.	4.0	11
53	Selective Protonation of Acidic Residues Triggers Opsin Activation. Journal of Physical Chemistry B, 2015, 119, 9510-9519.	1.2	15
54	The influence of alignment-free sequence representations on the semi-supervised classification of class C G protein-coupled receptors. Medical and Biological Engineering and Computing, 2015, 53, 137-149.	1.6	11

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55	Helix 3 acts as a conformational hinge in Class A GPCR activation: An analysis of interhelical interaction energies in crystal structures. Journal of Structural Biology, 2015, 192, 545-553.	1.3	18
56	Overlapping binding sites drive allosteric agonism and positive cooperativity in type 4 metabotropic glutamate receptors. FASEB Journal, 2015, 29, 116-130.	0.2	54
57	Follow-Up Genotoxic Study: Chromosome Damage Two and Six Years after Exposure to the Prestige Oil Spill. PLoS ONE, 2015, 10, e0132413.	1.1	14
58	Visual Characterization of Misclassified Class C GPCRs through Manifold-based Machine Learning Methods. Genomics and Computational Biology, 2015, 1, 19.	0.7	3
59	Reducing the n-gram feature space of class C GPCRs to subtype-discriminating patterns. Journal of Integrative Bioinformatics, 2014, 11, 99-115.	1.0	4
60	Visual interpretation of class C GPCR subtype overlapping from the nonlinear mapping of transformed primary sequences. , 2014, , .		4
61	Exploring the Active Conformation of Cyclohexane Carboxylate Positive Allosteric Modulators of the Typeâ€...4 Metabotropic Glutamate Receptor. ChemMedChem, 2014, 9, 2685-2698.	1.6	1
62	A double effect molecular switch leads to a novel potent negative allosteric modulator of metabotropic glutamate receptor 5. MedChemComm, 2014, 5, 1548-1554.	3.5	12
63	An allosteric modulator to control endogenous G protein-coupled receptors with light. Nature Chemical Biology, 2014, 10, 813-815.	3.9	147
64	Computational Analysis of Negative and Positive Allosteric Modulator Binding and Function in Metabotropic Glutamate Receptor 5 (In)Activation. Journal of Chemical Information and Modeling, 2014, 54, 1476-1487.	2.5	28
65	Finding Class C GPCR Subtype-Discriminating N-grams through Feature Selection. Advances in Intelligent Systems and Computing, 2014, , 89-96.	0.5	2
66	Mathematical Modeling of G Protein-Coupled Receptor Function: What Can We Learn from Empirical and Mechanistic Models?. Advances in Experimental Medicine and Biology, 2014, 796, 159-181.	0.8	7
67	Reducing the n-gram feature space of class C GPCRs to subtype-discriminating patterns. Journal of Integrative Bioinformatics, 2014, 11, 254.	1.0	1
68	Multiple active receptor conformation, agonist efficacy and maximum effect of the system: the conformation-based operational model of agonism. Drug Discovery Today, 2013, 18, 365-371.	3.2	10
69	Modeling Cooperativity Effects in Dimeric G Protein-Coupled Receptors. Progress in Molecular Biology and Translational Science, 2013, 115, 349-373.	0.9	7
70	Mechanistic analysis of the function of agonists and allosteric modulators: reconciling twoâ€state and operational models. British Journal of Pharmacology, 2013, 169, 1189-1202.	2.7	24
71	Detecting Loss of Diversity for an Efficient Termination of EAs. , 2013, , .		4
72	Chromosomal Bands Affected by Acute Oil Exposure and DNA Repair Errors. PLoS ONE, 2013, 8, e81276.	1.1	8

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73	Head Circumference Growth Function as a Marker of Neurological Impairment in a Cohort of Microcephalic Infants and Children. Neuropediatrics, 2012, 43, 271-274.	0.3	8
74	Pharmacological properties of S1RA, a new sigmaâ€1 receptor antagonist that inhibits neuropathic pain and activityâ€induced spinal sensitization. British Journal of Pharmacology, 2012, 166, 2289-2306.	2.7	159
75	Complementing Kernel-Based Visualization of Protein Sequences with Their Phylogenetic Tree. Lecture Notes in Computer Science, 2012, , 136-149.	1.0	3
76	Advanced age increases chromosome structural abnormalities in human spermatozoa. European Journal of Human Genetics, 2011, 19, 145-151.	1.4	42
77	Integrated Synthetic, Pharmacological, and Computational Investigation of cisâ€2â€(3,5â€Dichlorophenylcarbamoyl)cyclohexanecarboxylic Acid Enantiomers As Positive Allosteric Modulators of Metabotropic Glutamate Receptor Subtypeâ€…4. ChemMedChem, 2011, 6, 131-140.	1.6	9
78	A Genomewide Screen for Tolerance to Cationic Drugs Reveals Genes Important for Potassium Homeostasis in Saccharomyces cerevisiae. Eukaryotic Cell, 2011, 10, 1241-1250.	3.4	53
79	How inverse can a neutral antagonist be? Strategic questions after the rimonabant issue. Drug Discovery Today, 2010, 15, 411-415.	3.2	22
80	The asymmetric/symmetric activation of GPCR dimers as a possible mechanistic rationale for multiple signalling pathways. Trends in Pharmacological Sciences, 2010, 31, 15-21.	4.0	69
81	Evidence for Distinct Antagonist-Revealed Functional States of 5-Hydroxytryptamine_{2A}Receptor Homodimers. Molecular Pharmacology, 2009, 75, 1380-1391.	1.0	60
82	Modelling the interdependence between the stoichiometry of receptor oligomerization and ligand binding for a coexisting dimer/tetramer receptor system. British Journal of Pharmacology, 2009, 156, 28-35.	2.7	22
83	Coupling of the guanosine glycosidic bond conformation and the ribonucleotide cleavage reaction: Implications for barnase catalysis. Proteins: Structure, Function and Bioinformatics, 2008, 70, 415-428.	1.5	2
84	On the fitting of binding data when receptor dimerization is suspected. British Journal of Pharmacology, 2008, 155, 17-23.	2.7	28
85	Ecophysiological significance of scale-dependent patterns in prokaryotic genomes unveiled by a combination of statistic and genometric analyses. Genomics, 2008, 91, 538-543.	1.3	9
86	Modeling the Binding and Function of Metabotropic Glutamate Receptors. Journal of Pharmacology and Experimental Therapeutics, 2008, 325, 443-456.	1.3	24
87	Assessing Receptor Affinity for Inverse Agonists: Schild and Cheng-Prusoff Methods Revisited. Current Drug Targets, 2007, 8, 197-202.	1.0	21
88	Transient middle cerebral artery occlusion causes different structural, mechanical, and myogenic alterations in normotensive and hypertensive rats. American Journal of Physiology - Heart and Circulatory Physiology, 2007, 293, H628-H635.	1.5	34
89	The catalytic power of enzymes: Conformational selection or transition state stabilization?. FEBS Letters, 2006, 580, 2170-2177.	1.3	25
90	Chronic 5-HT6 receptor modulation by E-6837 induces hypophagia and sustained weight loss in diet-induced obese rats. British Journal of Pharmacology, 2006, 148, 973-983.	2.7	85

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91	Increased Superoxide Anion Production by Interleukin-1Î² Impairs Nitric Oxide-Mediated Relaxation in Resistance Arteries. Journal of Pharmacology and Experimental Therapeutics, 2006, 316, 42-52.	1.3	69
92	Chromosomal Instability in Amniocytes From Fetuses of Mothers Who Smoke. JAMA - Journal of the American Medical Association, 2005, 293, 1212.	3.8	75
93	Characterization of the Calcium-mediated Response to Alkaline Stress in Saccharomyces cerevisiae. Journal of Biological Chemistry, 2004, 279, 43614-43624.	1.6	180
94	Shift in nucleotide conformational equilibrium contributes to increased rate of catalysis of GpAp versus GpA in barnase. Proteins: Structure, Function and Bioinformatics, 2004, 56, 261-276.	1.5	6
95	Agonist induction, conformational selection, and mutant receptors. FEBS Letters, 2004, 556, 13-18.	1.3	13
96	Enhanced noradrenergic transmission in the spontaneously hypertensive rat anococcygeus muscle. British Journal of Pharmacology, 2003, 140, 773-779.	2.7	3
97	Role of Elastin in Spontaneously Hypertensive Rat Small Mesenteric Artery Remodelling. Journal of Physiology, 2003, 552, 185-195.	1.3	122
98	Empirical models and Hill coefficients. Trends in Pharmacological Sciences, 2003, 24, 63-65.	4.0	25
99	Assessing the (a)symmetry of concentration-effect curves. , 2002, 95, 21-45.		121
100	Changes in electrophysiological properties in the prostatic portion of vas deferens from spontaneously hypertensive rats. Naunyn-Schmiedeberg's Archives of Pharmacology, 2002, 366, 425-430.	1.4	4
101	Modelling the changes due to the endothelium and hypertension in the alpha-adenoreceptor-mediated responses of rat aorta. Autonomic and Autacoid Pharmacology, 1999, 19, 219-228.	0.7	17
102	Adrenergic and purinergic components in bisected vas deferens from spontaneously hypertensive rats. British Journal of Pharmacology, 1999, 128, 873-880.	2.7	7
103	A pH-dependent model of the activation mechanism of the histamine H2 receptor. Biochemical Pharmacology, 1999, 58, 343-353.	2.0	6
104	The slope parameter and the receptor reserve. Trends in Pharmacological Sciences, 1998, 19, 445.	4.0	5
105	Conformational analysis of GpA and GpAp in aqueous solution by molecular dynamics and statistical methods 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 1998, 283, 863-882.	2.0	6
106	The effect of the molecular mechanism of G protein-coupled receptor activation on the process of signal transduction. European Journal of Pharmacology, 1997, 335, 73-87.	1.7	11
107	Effects of l -NG -nitro-arginine on noradrenaline induced contraction in the rat anococcygeus muscle. British Journal of Pharmacology, 1997, 120, 1035-1038.	2.7	2
108	Î± 1 -Adrenoceptor vasoconstriction in the tail artery during ageing. British Journal of Pharmacology, 1997, 121, 1017-1023.	2.7	25

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109	Use of the operational model of agonism and [3H]prazosin binding to assess altered responsiveness of Î±1-adrenoceptors in the vas deferens of spontaneously hypertensive rat. Naunyn-Schmiedeberg's Archives of Pharmacology, 1997, 356, 383-391.	1.4	14
110	Effect of N^Gâ€nitroâ€Lâ€arginine methylester (Lâ€NAME) on functional and biochemical Î±₁â€adrenoceptorâ€mediated responses in rat blood vessels. British Journal of Pharmacology, 1996, 117, 757-763.	2.7	31
111	Endothelial modulation of Î±₁â€adrenoceptor contractile responses in the tail artery of spontaneously hypertensive rats. British Journal of Pharmacology, 1996, 119, 765-771.	2.7	15
112	Modelling the changes induced by chronic desipramine treatment on the factors governing the agonism at prejunctional Î±₂â€adrenoceptors. British Journal of Pharmacology, 1996, 117, 1286-1292.	2.7	5
113	The structure and activity of membrane receptors: computational simulation of histamine H2-receptor activation. Computational and Theoretical Chemistry, 1996, 371, 279-286.	1.5	2
114	Effect of nucleotide substrate binding on the pKa of catalytic residues in barnase. , 1996, 25, 180-194.		6
115	Analysis of agonism at functional prejunctional of rat vas deferens using operational and null approaches. European Journal of Pharmacology, 1994, 258, 229-238.	1.7	14
116	Kernel Generative Topographic Mapping of Protein Sequences. , 0, , 817-830.		0