Hugo GutiÃ©rrez de TerÃ¡n

List of Publications by Year
in descending order

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102 papers	2,691 citations	172207 29 h-index	223531 46 g-index
110 all docs	110 docs citations	110 times ranked	3409 citing authors

#	Article	IF	Citations
1	Optimization of 2-Amino-4,6-diarylpyrimidine-5-carbonitriles as Potent and Selective A1 Antagonists. Journal of Medicinal Chemistry, 2022, 65, 2091-2106.	2.9	2
2	Exploring Non-orthosteric Interactions with a Series of Potent and Selective A₃ Antagonists. ACS Medicinal Chemistry Letters, 2022, 13, 243-249.	1.3	3
3	Slow conformational dynamics of the human A2A adenosine receptor are temporally ordered. Structure, 2022, 30, 329-337.e5.	1.6	17
4	A_{2B}adenosine receptor antagonists rescue lymphocyte activity in adenosine-producing patient-derived cancer models. , 2022, 10, e004592.		8
5	N-(Methyloxycarbonyl)thiophene sulfonamides as high affinity AT2 receptor ligands. Bioorganic and Medicinal Chemistry, 2021, 29, 115859.	1.4	6
6	Design, synthesis, HER2 inhibition and anticancer evaluation of new substituted 1,5-dihydro-4,1-benzoxazepines. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 1551-1561.	2.5	6
7	Free Energy Calculations for Proteinâ€“Ligand Binding Prediction. Methods in Molecular Biology, 2021, 2266, 203-226.	0.4	11
8	Structural Basis of Inhibition of Human Insulin-Regulated Aminopeptidase (IRAP) by Benzopyran-Based Inhibitors. Frontiers in Molecular Biosciences, 2021, 8, 625274.	1.6	3
9	Editorial: Physiological, Pathological Roles and Pharmacology of Insulin Regulated Aminopeptidase. Frontiers in Molecular Biosciences, 2021, 8, 685101.	1.6	0
10	Potent and Subtype-Selective Dopamine D₂ Receptor Biased Partial Agonists Discovered via an Ugi-Based Approach. Journal of Medicinal Chemistry, 2021, 64, 8710-8726.	2.9	3
11	Identification of V6.51L as a selectivity hotspot in stereoselective A2B adenosine receptor antagonist recognition. Scientific Reports, 2021, 11, 14171.	1.6	11
12	Potent Inhibition of Nicotinamide N-Methyltransferase by Alkene-Linked Bisubstrate Mimics Bearing Electron Deficient Aromatics. Journal of Medicinal Chemistry, 2021, 64, 12938-12963.	2.9	43
13	3,4-Dihydropyrimidin-2(1H)-ones as Antagonists of the Human A_{2B} Adenosine Receptor: Optimization, Structureâ€“Activity Relationship Studies, and Enantiospecific Recognition. Journal of Medicinal Chemistry, 2021, 64, 458-480.	2.9	19
14	Deciphering conformational selectivity in the A2A adenosine G protein-coupled receptor by free energy simulations. PLoS Computational Biology, 2021, 17, e1009152.	1.5	5
15	Macrocyclic peptidomimetics as inhibitors of insulin-regulated aminopeptidase (IRAP). RSC Medicinal Chemistry, 2020, 11, 234-244.	1.7	9
16	GPCRmd uncovers the dynamics of the 3D-GPCRome. Nature Methods, 2020, 17, 777-787.	9.0	90
17	Xâ€Ray Crystallography and Free Energy Calculations Reveal the Binding Mechanism of A_{2A} Adenosine Receptor Antagonists. Angewandte Chemie - International Edition, 2020, 59, 16536-16543.	7.2	23
18	Nitrogen-Walk Approach to Explore Bioisosteric Replacements in a Series of Potent A_{2B} Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 2020, 63, 7721-7739.	2.9	20

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19	Synthesis, Evaluation and Proposed Binding Pose of Substituted Spiroâ€Oxindole Dihydroquinazolinones as IRAP Inhibitors. ChemistryOpen, 2020, 9, 325-337.	0.9	7
20	Xâ€Ray Crystallography and Free Energy Calculations Reveal the Binding Mechanism of A_{2A} Adenosine Receptor Antagonists. Angewandte Chemie, 2020, 132, 16679-16686.	1.6	1
21	Evolution of Angiotensin Peptides and Peptidomimetics as Angiotensin II Receptor Type 2 (AT2) Receptor Agonists. Biomolecules, 2020, 10, 649.	1.8	12
22	Characterization of cancer-related somatic mutations in the adenosine A2B receptor. European Journal of Pharmacology, 2020, 880, 173126.	1.7	15
23	Free-Energy Calculations for Bioisosteric Modifications of A3 Adenosine Receptor Antagonists. International Journal of Molecular Sciences, 2019, 20, 3499.	1.8	2
24	Inhibition of translation termination by small molecules targeting ribosomal release factors. Scientific Reports, 2019, 9, 15424.	1.6	6
25	QresFEP: An Automated Protocol for Free Energy Calculations of Protein Mutations in Q. Journal of Chemical Theory and Computation, 2019, 15, 5461-5473.	2.3	33
26	Trifluorinated Pyrimidine-Based A_{2B} Antagonists: Optimization and Evidence of Stereospecific Recognition. Journal of Medicinal Chemistry, 2019, 62, 9315-9330.	2.9	15
27	A Series of Analogues to the AT₂R Prototype Antagonist C38 Allow Fine Tuning of the Previously Reported Antagonist Binding Mode. ChemistryOpen, 2019, 8, 114-125.	0.9	8
28	Functional characterization in vitro of twelve naturally occurring variants of the human pancreatic polypeptide receptor NPY4R. Neuropeptides, 2019, 76, 101933.	0.9	3
29	QligFEP: an automated workflow for small molecule free energy calculations in Q. Journal of Cheminformatics, 2019, 11, 26.	2.8	51
30	Free energy calculations of RNA interactions. Methods, 2019, 162-163, 85-95.	1.9	7
31	Structural Basis of Inhibition of Human Insulin-Regulated Aminopeptidase (IRAP) by Aryl Sulfonamides. ACS Omega, 2018, 3, 4509-4521.	1.6	14
32	Elucidation of the Binding Mode of the Carboxyterminal Region of Peptide YY to the Human Y₂Receptor. Molecular Pharmacology, 2018, 93, 323-334.	1.0	28
33	Molecular Mechanisms in the Selectivity of Nonsteroidal Anti-Inflammatory Drugs. Biochemistry, 2018, 57, 1236-1248.	1.2	19
34	Q6: A comprehensive toolkit for empirical valence bond and related free energy calculations. SoftwareX, 2018, 7, 388-395.	1.2	47
35	Characterization of Ligand Binding to GPCRs Through Computational Methods. Methods in Molecular Biology, 2018, 1705, 23-44.	0.4	6
36	Structural Mapping of Adenosine Receptor Mutations: Ligand Binding and Signaling Mechanisms. Trends in Pharmacological Sciences, 2018, 39, 75-89.	4.0	64

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37	Structural mechanism of AadA, a dual-specificity aminoglycoside adenylyltransferase from Salmonella enterica. Journal of Biological Chemistry, 2018, 293, 11481-11490.	1.6	26
38	Exploring the influence of the substituent at position 4 in a series of 3,4-dihydropyrimidin-2(1H)-one A2B adenosine receptor antagonists. Chemistry of Heterocyclic Compounds, 2017, 53, 316-321.	0.6	7
39	3-Oxopyridazin-5-yl-Chalcone Hybrids: Potent Antiplatelet Agents That Prevent Glycoprotein IIb/IIIa Activation. ChemistrySelect, 2017, 2, 4920-4933.	0.7	4
40	Probing the Time Dependency of Cyclooxygenase-1 Inhibitors by Computer Simulations. Biochemistry, 2017, 56, 1911-1920.	1.2	5
41	A close-up view of codon selection in eukaryotic initiation. RNA Biology, 2017, 14, 815-819.	1.5	8
42	Enantiospecific Recognition at the A_{2B} Adenosine Receptor by Alkyl 2-Cyanoimino-4-substituted-6-methyl-1,2,3,4-tetrahydropyrimidine-5-carboxylates. Journal of Medicinal Chemistry, 2017, 60, 3372-3382.	2.9	26
43	The GPR139 reference agonists 1a and 7c, and tryptophan and phenylalanine share a common binding site. Scientific Reports, 2017, 7, 1128.	1.6	25
44	Effect of Nitrogen Atom Substitution in A₃ Adenosine Receptor Binding: N-(4,6-Diarylpyridin-2-yl)acetamides as Potent and Selective Antagonists. Journal of Medicinal Chemistry, 2017, 60, 7502-7511.	2.9	14
45	Structure-Based Design of Potent and Selective Ligands at the Four Adenosine Receptors. Molecules, 2017, 22, 1945.	1.7	30
46	Discovery of 7-(Prolinol-N-yl)-2-phenylamino-thiazolo[5,4-d]pyrimidines as Novel Non-Nucleoside Partial Agonists for the A2A Adenosine Receptor: Prediction from Molecular Modeling. Journal of Medicinal Chemistry, 2016, 59, 5922-5928.	2.9	23
47	Binding to and Inhibition of Insulin-Regulated Aminopeptidase by Macrocyclic Disulfides Enhances Spine Density. Molecular Pharmacology, 2016, 89, 413-424.	1.0	35
48	Aryl Sulfonamide Inhibitors of Insulin-Regulated Aminopeptidase Enhance Spine Density in Primary Hippocampal Neuron Cultures. ACS Chemical Neuroscience, 2016, 7, 1383-1392.	1.7	27
49	Computational exploration of the binding mode of hemeâ€dependent stimulators into the active catalytic domain of soluble guanylate cyclase. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1534-1548.	1.5	4
50	GPCR-ModSim: A comprehensive web based solution for modeling G-protein coupled receptors. Nucleic Acids Research, 2016, 44, W455-W462.	6.5	61
51	Discovery of Potent and Highly Selective A_{2B} Adenosine Receptor Antagonist Chemotypes. Journal of Medicinal Chemistry, 2016, 59, 1967-1983.	2.9	55
52	Structural determinants of subtype selectivity and functional activity of angiotensin II receptors. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 1355-1359.	1.0	15
53	Structure-Based Rational Design of Adenosine Receptor Ligands. Current Topics in Medicinal Chemistry, 2016, 17, 40-58.	1.0	29
54	Computational exploration of the binding mode of the heme-dependent activator YC-1 into the active catalytic site of soluble guanylate cyclase. BMC Pharmacology & Toxicology, 2015, 16, .	1.0	0

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55	Free energy calculations of A_{2A}adenosine receptor mutation effects on agonist binding. Chemical Communications, 2015, 51, 3522-3525.	2.2	33
56	New selective A_{2A}agonists and A₃antagonists for human adenosine receptors: synthesis, biological activity and molecular docking studies. MedChemComm, 2015, 6, 1178-1185.	3.5	9
57	Origin of the Enigmatic Stepwise Tight-Binding Inhibition of Cyclooxygenase-1. Biochemistry, 2015, 54, 7283-7291.	1.2	17
58	Sodium Ion Binding Pocket Mutations and Adenosine A_{2A}Receptor Function. Molecular Pharmacology, 2015, 87, 305-313.	1.0	79
59	Pyrazin-2(1H)-ones as a novel class of selective A3 adenosine receptor antagonists. Future Medicinal Chemistry, 2015, 7, 1373-1380.	1.1	8
60	Computer-Aided Design of GPCR Ligands. Methods in Molecular Biology, 2015, 1272, 271-291.	0.4	10
61	Computational Prediction of Alanine Scanning and Ligand Binding Energetics in G-Protein Coupled Receptors. PLoS Computational Biology, 2014, 10, e1003585.	1.5	58
62	Selective chaperone effect of aminocyclitol derivatives on G202R and other mutant glucocerebrosidases causing Gaucher disease. International Journal of Biochemistry and Cell Biology, 2014, 54, 245-254.	1.2	8
63	Toward an Optimal Docking and Free Energy Calculation Scheme in Ligand Design with Application to COX-1 Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 1488-1499.	2.5	20
64	Structureâ€Based Design of New KSPâ€Eg5 Inhibitors Assisted by a Targeted Multicomponent Reaction. ChemBioChem, 2014, 15, 1471-1480.	1.3	5
65	The roles of computational chemistry in the ligand design of G protein-coupled receptors: how far have we come and what should we expect?. Future Medicinal Chemistry, 2014, 6, 251-254.	1.1	6
66	Structural and Energetic Effects of A2A Adenosine Receptor Mutations on Agonist and Antagonist Binding. PLoS ONE, 2014, 9, e108492.	1.1	46
67	The Role of a Sodium Ion Binding Site in the Allosteric Modulation of the A2A Adenosine G Protein-Coupled Receptor. Structure, 2013, 21, 2175-2185.	1.6	118
68	Discovery of 3,4-Dihydropyrimidin-2(1H)-ones As a Novel Class of Potent and Selective A_{2B} Adenosine Receptor Antagonists. ACS Medicinal Chemistry Letters, 2013, 4, 1031-1036.	1.3	65
69	Characterization of the dynamic events of GPCRs by automated computational simulations. Biochemical Society Transactions, 2013, 41, 205-212.	1.6	40
70	Mutagenesis and Computational Modeling of Human G-Protein-Coupled Receptor Y2 for Neuropeptide Y and Peptide YY. Biochemistry, 2013, 52, 7987-7998.	1.2	23
71	Selective and potent adenosine A3 receptor antagonists by methoxyaryl substitution on the N-(2,6-diarylpyrimidin-4-yl)acetamide scaffold. European Journal of Medicinal Chemistry, 2013, 59, 235-242.	2.6	13
72	Computational Approaches for Ligand Discovery and Design in Class-A G Protein- Coupled Receptors. Current Pharmaceutical Design, 2013, 19, 2216-2236.	0.9	17

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73	Ligand-, structure- and pharmacophore-based molecular fingerprints: a case study on adenosine A1, A2A, A2B, and A3 receptor antagonists. Journal of Computer-Aided Molecular Design, 2012, 26, 1247-1266.	1.3	46
74	Linear Interaction Energy: Method and Applications in Drug Design. Methods in Molecular Biology, 2012, 819, 305-323.	0.4	78
75	Characterization of the homodimerization interface and functional hotspots of the CXCR4 chemokine receptor. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1919-1928.	1.5	33
76	Molecular Modelling of G Proteinâ€Coupled Receptors Through the Web. Molecular Informatics, 2012, 31, 334-341.	1.4	33
77	Computational Prediction of Structureâ^'Activity Relationships for the Binding of Aminocyclitols to Î²-Glucocerebrosidase. Journal of Chemical Information and Modeling, 2011, 51, 601-611.	2.5	14
78	Rational design of a cyclin A fluorescent peptide sensor. Organic and Biomolecular Chemistry, 2011, 9, 7629.	1.5	14
79	Molecular Dynamics Simulations Reveal Insights into Key Structural Elements of Adenosine Receptors. Biochemistry, 2011, 50, 4194-4208.	1.2	64
80	Pyrimidine Derivatives as Potent and Selective A₃ Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 2011, 54, 457-471.	2.9	56
81	Identification of positions in the human neuropeptide Y/peptide YY receptor Y2 that contribute to pharmacological differences between receptor subtypes. Neuropeptides, 2011, 45, 293-300.	0.9	13
82	In silico directed chemical probing of the adenosine receptor family. Bioorganic and Medicinal Chemistry, 2010, 18, 3043-3052.	1.4	28
83	Phe369(7.38) at human 5â€HT₇ receptors confers interspecies selectivity to antagonists and partial agonists. British Journal of Pharmacology, 2010, 159, 1069-1081.	2.7	13
84	Crystal structure of thioflavin-T and its binding to amyloid fibrils: insights at the molecular level. Chemical Communications, 2010, 46, 1156.	2.2	78
85	Mutagenesis of human neuropeptide Y/peptide YY receptor Y2 reveals additional differences to Y1 in interactions with highly conserved ligand positions. Regulatory Peptides, 2010, 163, 120-129.	1.9	15
86	A C-terminal mutation of ATP1A3 underscores the crucial role of sodium affinity in the pathophysiology of rapid-onset dystonia-parkinsonism. Human Molecular Genetics, 2009, 18, 2370-2377.	1.4	59
87	Identification of Novel Scaffolds from an Original Chemical Library as Potential Antipsychotics. QSAR and Combinatorial Science, 2009, 28, 856-860.	1.5	6
88	Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008. Nature Reviews Drug Discovery, 2009, 8, 455-463.	21.5	260
89	Î±-Substituted norstatines as the transition-state mimic in inhibitors of multiple digestive vacuole malaria aspartic proteases. Bioorganic and Medicinal Chemistry, 2009, 17, 5933-5949.	1.4	36
90	Recombinant Plasmepsin 1 from the Human Malaria Parasite Plasmodium falciparum: Enzymatic Characterization, Active Site Inhibitor Design, and Structural Analysis. Biochemistry, 2009, 48, 4086-4099.	1.2	20

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91	Synthesis, adenosine receptor binding and 3D-QSAR of 4-substituted 2-(2â€²-furyl)-1,2,4-triazolo[1,5-a]quinoxalines. Bioorganic and Medicinal Chemistry, 2008, 16, 2103-2113.	1.4	14
92	Computational inhibitor design against malaria plasmepsins. Cellular and Molecular Life Sciences, 2007, 64, 2285-2305.	2.4	43
93	Inhibitor Binding to the Plasmepsin IV Aspartic Protease from Plasmodium falciparum. Biochemistry, 2006, 45, 10529-10541.	1.2	28
94	Computational analysis of plasmepsin IV bound to an allophenylnorstatine inhibitor. FEBS Letters, 2006, 580, 5910-5916.	1.3	21
95	Macrocyclic inhibitors of the malarial aspartic proteases plasmepsin I, II, and IV. Bioorganic and Medicinal Chemistry, 2006, 14, 2197-2208.	1.4	39
96	Towards a MIP-based alignment and docking in computer-aided drug design. Proteins: Structure, Function and Bioinformatics, 2004, 56, 585-594.	1.5	6
97	Novel approaches for modeling of the A1 adenosine receptor and its agonist binding site. Proteins: Structure, Function and Bioinformatics, 2004, 54, 705-715.	1.5	23
98	Comparative Analysis of Putative Agonist-Binding Modes in the Human A1 Adenosine Receptor. ChemBioChem, 2004, 5, 841-849.	1.3	10
99	On the Generation of Catalytic Antibodies by Transition State Analogues. ChemBioChem, 2003, 4, 277-285.	1.3	29
100	Molecular Diversity Sample Generation on the Basis of Quantum-Mechanical Computations and Principal Component Analysis. Combinatorial Chemistry and High Throughput Screening, 2002, 5, 49-57.	0.6	3
101	Comparison of biomolecules on the basis of Molecular Interaction Potentials. Journal of the Brazilian Chemical Society, 2002, 13, 795-799.	0.6	10
102	Use of alignment-free molecular descriptors in diversity analysis and optimal sampling of molecular libraries. Molecular Diversity, 2000, 6, 135-147.	2.1	8