

Hugo Gutiérrez de Terán

List of Publications by Year in descending order

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102
papers

2,691
citations

172457

29
h-index

223800

46
g-index

110
all docs

110
docs citations

110
times ranked

3409
citing authors

#	ARTICLE	IF	CITATIONS
1	Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008. <i>Nature Reviews Drug Discovery</i> , 2009, 8, 455-463.	46.4	260
2	The Role of a Sodium Ion Binding Site in the Allosteric Modulation of the A2A Adenosine G Protein-Coupled Receptor. <i>Structure</i> , 2013, 21, 2175-2185.	3.3	118
3	GPCRmd uncovers the dynamics of the 3D-GPCRome. <i>Nature Methods</i> , 2020, 17, 777-787.	19.0	90
4	Sodium Ion Binding Pocket Mutations and Adenosine A _{2A} Receptor Function. <i>Molecular Pharmacology</i> , 2015, 87, 305-313.	2.3	79
5	Crystal structure of thioflavin-T and its binding to amyloid fibrils: insights at the molecular level. <i>Chemical Communications</i> , 2010, 46, 1156.	4.1	78
6	Linear Interaction Energy: Method and Applications in Drug Design. <i>Methods in Molecular Biology</i> , 2012, 819, 305-323.	0.9	78
7	Discovery of 3,4-Dihydropyrimidin-2(1 <i>H</i>)-ones As a Novel Class of Potent and Selective A _{2B} Adenosine Receptor Antagonists. <i>ACS Medicinal Chemistry Letters</i> , 2013, 4, 1031-1036.	2.8	65
8	Molecular Dynamics Simulations Reveal Insights into Key Structural Elements of Adenosine Receptors. <i>Biochemistry</i> , 2011, 50, 4194-4208.	2.5	64
9	Structural Mapping of Adenosine Receptor Mutations: Ligand Binding and Signaling Mechanisms. <i>Trends in Pharmacological Sciences</i> , 2018, 39, 75-89.	8.7	64
10	GPCR-ModSim: A comprehensive web based solution for modeling G-protein coupled receptors. <i>Nucleic Acids Research</i> , 2016, 44, W455-W462.	14.5	61
11	A C-terminal mutation of ATP1A3 underscores the crucial role of sodium affinity in the pathophysiology of rapid-onset dystonia-parkinsonism. <i>Human Molecular Genetics</i> , 2009, 18, 2370-2377.	2.9	59
12	Computational Prediction of Alanine Scanning and Ligand Binding Energetics in G-Protein Coupled Receptors. <i>PLoS Computational Biology</i> , 2014, 10, e1003585.	3.2	58
13	Pyrimidine Derivatives as Potent and Selective A ₃ Adenosine Receptor Antagonists. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 457-471.	6.4	56
14	Discovery of Potent and Highly Selective A _{2B} Adenosine Receptor Antagonist Chemotypes. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 1967-1983.	6.4	55
15	QligFEP: an automated workflow for small molecule free energy calculations in Q. <i>Journal of Cheminformatics</i> , 2019, 11, 26.	6.1	51
16	Q6: A comprehensive toolkit for empirical valence bond and related free energy calculations. <i>SoftwareX</i> , 2018, 7, 388-395.	2.6	47
17	Ligand-, structure- and pharmacophore-based molecular fingerprints: a case study on adenosine A1, A2A, A2B, and A3 receptor antagonists. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 1247-1266.	2.9	46
18	Structural and Energetic Effects of A2A Adenosine Receptor Mutations on Agonist and Antagonist Binding. <i>PLoS ONE</i> , 2014, 9, e108492.	2.5	46

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19	Computational inhibitor design against malaria plasmepsins. Cellular and Molecular Life Sciences, 2007, 64, 2285-2305.	5.4	43
20	Potent Inhibition of Nicotinamide <i>N</i> -Methyltransferase by Alkene-Linked Bisubstrate Mimics Bearing Electron Deficient Aromatics. Journal of Medicinal Chemistry, 2021, 64, 12938-12963.	6.4	43
21	Characterization of the dynamic events of GPCRs by automated computational simulations. Biochemical Society Transactions, 2013, 41, 205-212.	3.4	40
22	Macrocyclic inhibitors of the malarial aspartic proteases plasmepsin I, II, and IV. Bioorganic and Medicinal Chemistry, 2006, 14, 2197-2208.	3.0	39
23	Î±-Substituted norstatins as the transition-state mimic in inhibitors of multiple digestive vacuole malaria aspartic proteases. Bioorganic and Medicinal Chemistry, 2009, 17, 5933-5949.	3.0	36
24	Binding to and Inhibition of Insulin-Regulated Aminopeptidase by Macrocyclic Disulfides Enhances Spine Density. Molecular Pharmacology, 2016, 89, 413-424.	2.3	35
25	Characterization of the homodimerization interface and functional hotspots of the CXCR4 chemokine receptor. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1919-1928.	2.6	33
26	Molecular Modelling of G Proteinâ€‘Coupled Receptors Through the Web. Molecular Informatics, 2012, 31, 334-341.	2.5	33
27	Free energy calculations of A _{2A} adenosine receptor mutation effects on agonist binding. Chemical Communications, 2015, 51, 3522-3525.	4.1	33
28	QresFEP: An Automated Protocol for Free Energy Calculations of Protein Mutations in Q. Journal of Chemical Theory and Computation, 2019, 15, 5461-5473.	5.3	33
29	Structure-Based Design of Potent and Selective Ligands at the Four Adenosine Receptors. Molecules, 2017, 22, 1945.	3.8	30
30	On the Generation of Catalytic Antibodies by Transition State Analogues. ChemBioChem, 2003, 4, 277-285.	2.6	29
31	Structure-Based Rational Design of Adenosine Receptor Ligands. Current Topics in Medicinal Chemistry, 2016, 17, 40-58.	2.1	29
32	Inhibitor Binding to the Plasmepsin IV Aspartic Protease from Plasmodium falciparum. Biochemistry, 2006, 45, 10529-10541.	2.5	28
33	In silico directed chemical probing of the adenosine receptor family. Bioorganic and Medicinal Chemistry, 2010, 18, 3043-3052.	3.0	28
34	Elucidation of the Binding Mode of the Carboxyterminal Region of Peptide YY to the Human Y ₂ Receptor. Molecular Pharmacology, 2018, 93, 323-334.	2.3	28
35	Aryl Sulfonamide Inhibitors of Insulin-Regulated Aminopeptidase Enhance Spine Density in Primary Hippocampal Neuron Cultures. ACS Chemical Neuroscience, 2016, 7, 1383-1392.	3.5	27
36	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.	6.4	26

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37	Structural mechanism of AadA, a dual-specificity aminoglycoside adenylyltransferase from <i>Salmonella enterica</i> . <i>Journal of Biological Chemistry</i> , 2018, 293, 11481-11490.	3.4	26
38	The GPR139 reference agonists 1a and 7c, and tryptophan and phenylalanine share a common binding site. <i>Scientific Reports</i> , 2017, 7, 1128.	3.3	25
39	Novel approaches for modeling of the A1 adenosine receptor and its agonist binding site. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 54, 705-715.	2.6	23
40	Mutagenesis and Computational Modeling of Human G-Protein-Coupled Receptor Y2 for Neuropeptide Y and Peptide YY. <i>Biochemistry</i> , 2013, 52, 7987-7998.	2.5	23
41	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. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 5922-5928.	6.4	23
42	X-ray Crystallography and Free Energy Calculations Reveal the Binding Mechanism of A _{2A} Adenosine Receptor Antagonists. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 16536-16543.	13.8	23
43	Computational analysis of plasmepsin IV bound to an allophenylnorstatine inhibitor. <i>FEBS Letters</i> , 2006, 580, 5910-5916.	2.8	21
44	Recombinant Plasmepsin 1 from the Human Malaria Parasite <i>Plasmodium falciparum</i> : Enzymatic Characterization, Active Site Inhibitor Design, and Structural Analysis. <i>Biochemistry</i> , 2009, 48, 4086-4099.	2.5	20
45	Toward an Optimal Docking and Free Energy Calculation Scheme in Ligand Design with Application to COX-1 Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1488-1499.	5.4	20
46	Nitrogen-Walk Approach to Explore Bioisosteric Replacements in a Series of Potent A _{2B} Adenosine Receptor Antagonists. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 7721-7739.	6.4	20
47	Molecular Mechanisms in the Selectivity of Nonsteroidal Anti-Inflammatory Drugs. <i>Biochemistry</i> , 2018, 57, 1236-1248.	2.5	19
48	3,4-Dihydropyrimidin-2(1 <i>H</i>)-ones as Antagonists of the Human A _{2B} Adenosine Receptor: Optimization, Structure-Activity Relationship Studies, and Enantiospecific Recognition. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 458-480.	6.4	19
49	Computational Approaches for Ligand Discovery and Design in Class-A G Protein-Coupled Receptors. <i>Current Pharmaceutical Design</i> , 2013, 19, 2216-2236.	1.9	17
50	Origin of the Enigmatic Stepwise Tight-Binding Inhibition of Cyclooxygenase-1. <i>Biochemistry</i> , 2015, 54, 7283-7291.	2.5	17
51	Slow conformational dynamics of the human A2A adenosine receptor are temporally ordered. <i>Structure</i> , 2022, 30, 329-337.e5.	3.3	17
52	Mutagenesis of human neuropeptide Y/peptide YY receptor Y2 reveals additional differences to Y1 in interactions with highly conserved ligand positions. <i>Regulatory Peptides</i> , 2010, 163, 120-129.	1.9	15
53	Structural determinants of subtype selectivity and functional activity of angiotensin II receptors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2016, 26, 1355-1359.	2.2	15
54	Trifluorinated Pyrimidine-Based A _{2B} Antagonists: Optimization and Evidence of Stereospecific Recognition. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 9315-9330.	6.4	15

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55	Characterization of cancer-related somatic mutations in the adenosine A2B receptor. <i>European Journal of Pharmacology</i> , 2020, 880, 173126.	3.5	15
56	Synthesis, adenosine receptor binding and 3D-QSAR of 4-substituted 2-(2-furyl)-1,2,4-triazolo[1,5-a]quinoxalines. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 2103-2113.	3.0	14
57	Computational Prediction of Structure-Activity Relationships for the Binding of Aminocyclitols to β -Glucocerebrosidase. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 601-611.	5.4	14
58	Rational design of a cyclin A fluorescent peptide sensor. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 7629.	2.8	14
59	Effect of Nitrogen Atom Substitution in A ₃ Adenosine Receptor Binding: <i>N</i> -(4,6-Diarylpyridin-2-yl)acetamides as Potent and Selective Antagonists. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 7502-7511.	6.4	14
60	Structural Basis of Inhibition of Human Insulin-Regulated Aminopeptidase (IRAP) by Aryl Sulfonamides. <i>ACS Omega</i> , 2018, 3, 4509-4521.	3.5	14
61	Phe369(7.38) at human 5-HT ₇ receptors confers interspecies selectivity to antagonists and partial agonists. <i>British Journal of Pharmacology</i> , 2010, 159, 1069-1081.	5.4	13
62	Identification of positions in the human neuropeptide Y/peptide YY receptor Y2 that contribute to pharmacological differences between receptor subtypes. <i>Neuropeptides</i> , 2011, 45, 293-300.	2.2	13
63	Selective and potent adenosine A3 receptor antagonists by methoxyaryl substitution on the N-(2,6-diarylpyrimidin-4-yl)acetamide scaffold. <i>European Journal of Medicinal Chemistry</i> , 2013, 59, 235-242.	5.5	13
64	Evolution of Angiotensin Peptides and Peptidomimetics as Angiotensin II Receptor Type 2 (AT2) Receptor Agonists. <i>Biomolecules</i> , 2020, 10, 649.	4.0	12
65	Free Energy Calculations for Protein-Ligand Binding Prediction. <i>Methods in Molecular Biology</i> , 2021, 2266, 203-226.	0.9	11
66	Identification of V6.51L as a selectivity hotspot in stereoselective A2B adenosine receptor antagonist recognition. <i>Scientific Reports</i> , 2021, 11, 14171.	3.3	11
67	Comparative Analysis of Putative Agonist-Binding Modes in the Human A1 Adenosine Receptor. <i>ChemBioChem</i> , 2004, 5, 841-849.	2.6	10
68	Computer-Aided Design of GPCR Ligands. <i>Methods in Molecular Biology</i> , 2015, 1272, 271-291.	0.9	10
69	Comparison of biomolecules on the basis of Molecular Interaction Potentials. <i>Journal of the Brazilian Chemical Society</i> , 2002, 13, 795-799.	0.6	10
70	New selective A _{2A} agonists and A ₃ antagonists for human adenosine receptors: synthesis, biological activity and molecular docking studies. <i>MedChemComm</i> , 2015, 6, 1178-1185.	3.4	9
71	Macrocyclic peptidomimetics as inhibitors of insulin-regulated aminopeptidase (IRAP). <i>RSC Medicinal Chemistry</i> , 2020, 11, 234-244.	3.9	9
72	Use of alignment-free molecular descriptors in diversity analysis and optimal sampling of molecular libraries. <i>Molecular Diversity</i> , 2000, 6, 135-147.	3.9	8

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73	Selective chaperone effect of aminocyclitol derivatives on G202R and other mutant glucocerebrosidases causing Gaucher disease. <i>International Journal of Biochemistry and Cell Biology</i> , 2014, 54, 245-254.	2.8	8
74	Pyrazin-2(1 <i>H</i>)-ones as a novel class of selective A3 adenosine receptor antagonists. <i>Future Medicinal Chemistry</i> , 2015, 7, 1373-1380.	2.3	8
75	A close-up view of codon selection in eukaryotic initiation. <i>RNA Biology</i> , 2017, 14, 815-819.	3.1	8
76	A Series of Analogues to the AT ₂ R Prototype Antagonist C38 Allow Fine Tuning of the Previously Reported Antagonist Binding Mode. <i>ChemistryOpen</i> , 2019, 8, 114-125.	1.9	8
77	A _{2B} adenosine receptor antagonists rescue lymphocyte activity in adenosine-producing patient-derived cancer models. , 2022, 10, e004592.		8
78	Exploring the influence of the substituent at position 4 in a series of 3,4-dihydropyrimidin-2(1 <i>H</i>)-one A2B adenosine receptor antagonists. <i>Chemistry of Heterocyclic Compounds</i> , 2017, 53, 316-321.	1.2	7
79	Free energy calculations of RNA interactions. <i>Methods</i> , 2019, 162-163, 85-95.	3.8	7
80	Synthesis, Evaluation and Proposed Binding Pose of Substituted Spirooxindole Dihydroquinazolinones as IRAP Inhibitors. <i>ChemistryOpen</i> , 2020, 9, 325-337.	1.9	7
81	Towards a MIP-based alignment and docking in computer-aided drug design. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 56, 585-594.	2.6	6
82	Identification of Novel Scaffolds from an Original Chemical Library as Potential Antipsychotics. <i>QSAR and Combinatorial Science</i> , 2009, 28, 856-860.	1.4	6
83	The roles of computational chemistry in the ligand design of G protein-coupled receptors: how far have we come and what should we expect?. <i>Future Medicinal Chemistry</i> , 2014, 6, 251-254.	2.3	6
84	Characterization of Ligand Binding to GPCRs Through Computational Methods. <i>Methods in Molecular Biology</i> , 2018, 1705, 23-44.	0.9	6
85	Inhibition of translation termination by small molecules targeting ribosomal release factors. <i>Scientific Reports</i> , 2019, 9, 15424.	3.3	6
86	N-(Methyloxycarbonyl)thiophene sulfonamides as high affinity AT2 receptor ligands. <i>Bioorganic and Medicinal Chemistry</i> , 2021, 29, 115859.	3.0	6
87	Design, synthesis, HER2 inhibition and anticancer evaluation of new substituted 1,5-dihydro-4,1-benzoxazepines. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2021, 36, 1551-1561.	5.2	6
88	Structure-Based Design of New KSP ^{Eg5} Inhibitors Assisted by a Targeted Multicomponent Reaction. <i>ChemBioChem</i> , 2014, 15, 1471-1480.	2.6	5
89	Probing the Time Dependency of Cyclooxygenase-1 Inhibitors by Computer Simulations. <i>Biochemistry</i> , 2017, 56, 1911-1920.	2.5	5
90	Deciphering conformational selectivity in the A2A adenosine G protein-coupled receptor by free energy simulations. <i>PLoS Computational Biology</i> , 2021, 17, e1009152.	3.2	5

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91	Computational exploration of the binding mode of heme-dependent stimulators into the active catalytic domain of soluble guanylate cyclase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 1534-1548.	2.6	4
92	3-Oxopyridazin-5-yl-Chalcone Hybrids: Potent Antiplatelet Agents That Prevent Glycoprotein IIb/IIIa Activation. <i>ChemistrySelect</i> , 2017, 2, 4920-4933.	1.5	4
93	Molecular Diversity Sample Generation on the Basis of Quantum-Mechanical Computations and Principal Component Analysis. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2002, 5, 49-57.	1.1	3
94	Functional characterization in vitro of twelve naturally occurring variants of the human pancreatic polypeptide receptor NPY4R. <i>Neuropeptides</i> , 2019, 76, 101933.	2.2	3
95	Structural Basis of Inhibition of Human Insulin-Regulated Aminopeptidase (IRAP) by Benzopyran-Based Inhibitors. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 625274.	3.5	3
96	Potent and Subtype-Selective Dopamine D ₂ Receptor Biased Partial Agonists Discovered via an Ugi-Based Approach. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 8710-8726.	6.4	3
97	Exploring Non-orthosteric Interactions with a Series of Potent and Selective A ₃ Antagonists. <i>ACS Medicinal Chemistry Letters</i> , 2022, 13, 243-249.	2.8	3
98	Free-Energy Calculations for Bioisosteric Modifications of A ₃ Adenosine Receptor Antagonists. <i>International Journal of Molecular Sciences</i> , 2019, 20, 3499.	4.1	2
99	Optimization of 2-Amino-4,6-diarylpyrimidine-5-carbonitriles as Potent and Selective A ₁ Antagonists. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 2091-2106.	6.4	2
100	X-Ray Crystallography and Free Energy Calculations Reveal the Binding Mechanism of A _{2A} Adenosine Receptor Antagonists. <i>Angewandte Chemie</i> , 2020, 132, 16679-16686.	2.0	1
101	Computational exploration of the binding mode of the heme-dependent activator YC-1 into the active catalytic site of soluble guanylate cyclase. <i>BMC Pharmacology & Toxicology</i> , 2015, 16, .	2.4	0
102	Editorial: Physiological, Pathological Roles and Pharmacology of Insulin Regulated Aminopeptidase. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 685101.	3.5	0