

Hugo Gutiérrez de Terán

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	Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008. <i>Nature Reviews Drug Discovery</i> , 2009, 8, 455-463.	21.5	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.	1.6	118
3	GPCRmd uncovers the dynamics of the 3D-GPCRome. <i>Nature Methods</i> , 2020, 17, 777-787.	9.0	90
4	Sodium Ion Binding Pocket Mutations and Adenosine A _{2A} Receptor Function. <i>Molecular Pharmacology</i> , 2015, 87, 305-313.	1.0	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.	2.2	78
6	Linear Interaction Energy: Method and Applications in Drug Design. <i>Methods in Molecular Biology</i> , 2012, 819, 305-323.	0.4	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.	1.3	65
8	Molecular Dynamics Simulations Reveal Insights into Key Structural Elements of Adenosine Receptors. <i>Biochemistry</i> , 2011, 50, 4194-4208.	1.2	64
9	Structural Mapping of Adenosine Receptor Mutations: Ligand Binding and Signaling Mechanisms. <i>Trends in Pharmacological Sciences</i> , 2018, 39, 75-89.	4.0	64
10	GPCR-ModSim: A comprehensive web based solution for modeling G-protein coupled receptors. <i>Nucleic Acids Research</i> , 2016, 44, W455-W462.	6.5	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.	1.4	59
12	Computational Prediction of Alanine Scanning and Ligand Binding Energetics in G-Protein Coupled Receptors. <i>PLoS Computational Biology</i> , 2014, 10, e1003585.	1.5	58
13	Pyrimidine Derivatives as Potent and Selective A ₃ Adenosine Receptor Antagonists. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 457-471.	2.9	56
14	Discovery of Potent and Highly Selective A _{2B} Adenosine Receptor Antagonist Chemotypes. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 1967-1983.	2.9	55
15	QligFEP: an automated workflow for small molecule free energy calculations in Q. <i>Journal of Cheminformatics</i> , 2019, 11, 26.	2.8	51
16	Q6: A comprehensive toolkit for empirical valence bond and related free energy calculations. <i>SoftwareX</i> , 2018, 7, 388-395.	1.2	47
17	Ligand-, structure- and pharmacophore-based molecular fingerprints: a case study on adenosine A ₁ , A _{2A} , A _{2B} , and A ₃ receptor antagonists. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 1247-1266.	1.3	46
18	Structural and Energetic Effects of A _{2A} Adenosine Receptor Mutations on Agonist and Antagonist Binding. <i>PLoS ONE</i> , 2014, 9, e108492.	1.1	46

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19	Computational inhibitor design against malaria plasmepsins. <i>Cellular and Molecular Life Sciences</i> , 2007, 64, 2285-2305.	2.4	43
20	Potent Inhibition of Nicotinamide <i>N</i> -Methyltransferase by Alkene-Linked Bisubstrate Mimics Bearing Electron Deficient Aromatics. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 12938-12963.	2.9	43
21	Characterization of the dynamic events of GPCRs by automated computational simulations. <i>Biochemical Society Transactions</i> , 2013, 41, 205-212.	1.6	40
22	Macrocyclic inhibitors of the malarial aspartic proteases plasmepsin I, II, and IV. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 2197-2208.	1.4	39
23	Î±-Substituted norstatins as the transition-state mimic in inhibitors of multiple digestive vacuole malaria aspartic proteases. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 5933-5949.	1.4	36
24	Binding to and Inhibition of Insulin-Regulated Aminopeptidase by Macrocyclic Disulfides Enhances Spine Density. <i>Molecular Pharmacology</i> , 2016, 89, 413-424.	1.0	35
25	Characterization of the homodimerization interface and functional hotspots of the CXCR4 chemokine receptor. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 1919-1928.	1.5	33
26	Molecular Modelling of G Proteinâ€Coupled Receptors Through the Web. <i>Molecular Informatics</i> , 2012, 31, 334-341.	1.4	33
27	Free energy calculations of A _{2A} adenosine receptor mutation effects on agonist binding. <i>Chemical Communications</i> , 2015, 51, 3522-3525.	2.2	33
28	QresFEP: An Automated Protocol for Free Energy Calculations of Protein Mutations in Q. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5461-5473.	2.3	33
29	Structure-Based Design of Potent and Selective Ligands at the Four Adenosine Receptors. <i>Molecules</i> , 2017, 22, 1945.	1.7	30
30	On the Generation of Catalytic Antibodies by Transition State Analogues. <i>ChemBioChem</i> , 2003, 4, 277-285.	1.3	29
31	Structure-Based Rational Design of Adenosine Receptor Ligands. <i>Current Topics in Medicinal Chemistry</i> , 2016, 17, 40-58.	1.0	29
32	Inhibitor Binding to the Plasmepsin IV Aspartic Protease from <i>Plasmodium falciparum</i> . <i>Biochemistry</i> , 2006, 45, 10529-10541.	1.2	28
33	In silico directed chemical probing of the adenosine receptor family. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 3043-3052.	1.4	28
34	Elucidation of the Binding Mode of the Carboxyterminal Region of Peptide YY to the Human Y ₂ Receptor. <i>Molecular Pharmacology</i> , 2018, 93, 323-334.	1.0	28
35	Aryl Sulfonamide Inhibitors of Insulin-Regulated Aminopeptidase Enhance Spine Density in Primary Hippocampal Neuron Cultures. <i>ACS Chemical Neuroscience</i> , 2016, 7, 1383-1392.	1.7	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. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 3372-3382.	2.9	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.	1.6	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.	1.6	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.	1.5	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.	1.2	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.	2.9	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.	7.2	23
43	Computational analysis of plasmepsin IV bound to an allophenylnorstatine inhibitor. <i>FEBS Letters</i> , 2006, 580, 5910-5916.	1.3	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.	1.2	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.	2.5	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.	2.9	20
47	Molecular Mechanisms in the Selectivity of Nonsteroidal Anti-Inflammatory Drugs. <i>Biochemistry</i> , 2018, 57, 1236-1248.	1.2	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.	2.9	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.	0.9	17
50	Origin of the Enigmatic Stepwise Tight-Binding Inhibition of Cyclooxygenase-1. <i>Biochemistry</i> , 2015, 54, 7283-7291.	1.2	17
51	Slow conformational dynamics of the human A2A adenosine receptor are temporally ordered. <i>Structure</i> , 2022, 30, 329-337.e5.	1.6	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.	1.0	15
54	Trifluorinated Pyrimidine-Based A _{2B} Antagonists: Optimization and Evidence of Stereospecific Recognition. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 9315-9330.	2.9	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.	1.7	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.	1.4	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.	2.5	14
58	Rational design of a cyclin A fluorescent peptide sensor. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 7629.	1.5	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.	2.9	14
60	Structural Basis of Inhibition of Human Insulin-Regulated Aminopeptidase (IRAP) by Aryl Sulfonamides. <i>ACS Omega</i> , 2018, 3, 4509-4521.	1.6	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.	2.7	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.	0.9	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.	2.6	13
64	Evolution of Angiotensin Peptides and Peptidomimetics as Angiotensin II Receptor Type 2 (AT2) Receptor Agonists. <i>Biomolecules</i> , 2020, 10, 649.	1.8	12
65	Free Energy Calculations for Protein-Ligand Binding Prediction. <i>Methods in Molecular Biology</i> , 2021, 2266, 203-226.	0.4	11
66	Identification of V6.51L as a selectivity hotspot in stereoselective A2B adenosine receptor antagonist recognition. <i>Scientific Reports</i> , 2021, 11, 14171.	1.6	11
67	Comparative Analysis of Putative Agonist-Binding Modes in the Human A1 Adenosine Receptor. <i>ChemBioChem</i> , 2004, 5, 841-849.	1.3	10
68	Computer-Aided Design of GPCR Ligands. <i>Methods in Molecular Biology</i> , 2015, 1272, 271-291.	0.4	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.	3.5	9
71	Macrocyclic peptidomimetics as inhibitors of insulin-regulated aminopeptidase (IRAP). <i>RSC Medicinal Chemistry</i> , 2020, 11, 234-244.	1.7	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.	2.1	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.	1.2	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.	1.1	8
75	A close-up view of codon selection in eukaryotic initiation. <i>RNA Biology</i> , 2017, 14, 815-819.	1.5	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.	0.9	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.	0.6	7
79	Free energy calculations of RNA interactions. <i>Methods</i> , 2019, 162-163, 85-95.	1.9	7
80	Synthesis, Evaluation and Proposed Binding Pose of Substituted Spirooxindole Dihydroquinazolinones as IRAP Inhibitors. <i>ChemistryOpen</i> , 2020, 9, 325-337.	0.9	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.	1.5	6
82	Identification of Novel Scaffolds from an Original Chemical Library as Potential Antipsychotics. <i>QSAR and Combinatorial Science</i> , 2009, 28, 856-860.	1.5	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.	1.1	6
84	Characterization of Ligand Binding to GPCRs Through Computational Methods. <i>Methods in Molecular Biology</i> , 2018, 1705, 23-44.	0.4	6
85	Inhibition of translation termination by small molecules targeting ribosomal release factors. <i>Scientific Reports</i> , 2019, 9, 15424.	1.6	6
86	N-(Methyloxycarbonyl)thiophene sulfonamides as high affinity AT2 receptor ligands. <i>Bioorganic and Medicinal Chemistry</i> , 2021, 29, 115859.	1.4	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.	2.5	6
88	Structure-Based Design of New KSP ^{Eg5} Inhibitors Assisted by a Targeted Multicomponent Reaction. <i>ChemBioChem</i> , 2014, 15, 1471-1480.	1.3	5
89	Probing the Time Dependency of Cyclooxygenase-1 Inhibitors by Computer Simulations. <i>Biochemistry</i> , 2017, 56, 1911-1920.	1.2	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.	1.5	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.	1.5	4
92	3-Oxopyridazin-5-yl-Chalcone Hybrids: Potent Antiplatelet Agents That Prevent Glycoprotein IIb/IIIa Activation. <i>ChemistrySelect</i> , 2017, 2, 4920-4933.	0.7	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.	0.6	3
94	Functional characterization in vitro of twelve naturally occurring variants of the human pancreatic polypeptide receptor NPY4R. <i>Neuropeptides</i> , 2019, 76, 101933.	0.9	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.	1.6	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.	2.9	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.	1.3	3
98	Free-Energy Calculations for Bioisosteric Modifications of A ₃ Adenosine Receptor Antagonists. <i>International Journal of Molecular Sciences</i> , 2019, 20, 3499.	1.8	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.	2.9	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.	1.6	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, .	1.0	0
102	Editorial: Physiological, Pathological Roles and Pharmacology of Insulin Regulated Aminopeptidase. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 685101.	1.6	0