Willem Jespers

List of Publications by Year in descending order

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27 papers	564 citations	623188 14 h-index	642321 23 g-index
30 all docs	30 docs citations	30 times ranked	633 citing authors

#	Article	IF	Citations
1	GPCRmd uncovers the dynamics of the 3D-GPCRome. Nature Methods, 2020, 17, 777-787.	9.0	90
2	Structural Mapping of Adenosine Receptor Mutations: Ligand Binding and Signaling Mechanisms. Trends in Pharmacological Sciences, 2018, 39, 75-89.	4.0	64
3	QligFEP: an automated workflow for small molecule free energy calculations in Q. Journal of Cheminformatics, 2019, 11, 26.	2.8	51
4	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
5	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
6	Theoretical Infrared Spectra: Quantitative Similarity Measures and Force Fields. Journal of Chemical Theory and Computation, 2020, 16, 3307-3315.	2.3	31
7	Structure-Based Design of Potent and Selective Ligands at the Four Adenosine Receptors. Molecules, 2017, 22, 1945.	1.7	30
8	The GPR139 reference agonists 1a and 7c, and tryptophan and phenylalanine share a common binding site. Scientific Reports, 2017, 7, 1128.	1.6	25
9	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
10	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
11	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
12	Novel Cephalosporin Conjugates Display Potent and Selective Inhibition of Imipenemase-Type Metallo-Î²-Lactamases. Journal of Medicinal Chemistry, 2021, 64, 9141-9151.	2.9	16
13	Trifluorinated Pyrimidine-Based A_{2B} Antagonists: Optimization and Evidence of Stereospecific Recognition. Journal of Medicinal Chemistry, 2019, 62, 9315-9330.	2.9	15
14	Characterization of cancer-related somatic mutations in the adenosine A2B receptor. European Journal of Pharmacology, 2020, 880, 173126.	1.7	15
15	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
16	Interacting with GPCRs: Using Interaction Fingerprints for Virtual Screening. Journal of Chemical Information and Modeling, 2016, 56, 2053-2060.	2.5	12
17	Free Energy Calculations for Proteinâ€“Ligand Binding Prediction. Methods in Molecular Biology, 2021, 2266, 203-226.	0.4	11
18	Identification of V6.51L as a selectivity hotspot in stereoselective A2B adenosine receptor antagonist recognition. Scientific Reports, 2021, 11, 14171.	1.6	11

#	Article	IF	Citations
19	A_{2B}adenosine receptor antagonists rescue lymphocyte activity in adenosine-producing patient-derived cancer models. , 2022, 10, e004592.		8
20	Free energy calculations of RNA interactions. Methods, 2019, 162-163, 85-95.	1.9	7
21	Characterization of Ligand Binding to GPCRs Through Computational Methods. Methods in Molecular Biology, 2018, 1705, 23-44.	0.4	6
22	Deciphering conformational selectivity in the A2A adenosine G protein-coupled receptor by free energy simulations. PLoS Computational Biology, 2021, 17, e1009152.	1.5	5
23	Successive Statistical and Structure-Based Modeling to Identify Chemically Novel Kinase Inhibitors. Journal of Chemical Information and Modeling, 2020, 60, 4283-4295.	2.5	4
24	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
25	Free-Energy Calculations for Bioisosteric Modifications of A3 Adenosine Receptor Antagonists. International Journal of Molecular Sciences, 2019, 20, 3499.	1.8	2
26	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
27	Cancer-Related Somatic Mutations in Transmembrane Helices Alter Adenosine A1 Receptor Pharmacology. Molecules, 2022, 27, 3742.	1.7	1