

Jens Carlsson

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

61
papers

2,619
citations

28
h-index

50
g-index

66
ext. papers

3,151
ext. citations

8
avg, IF

5.13
L-index

#	Paper	IF	Citations
61	Ultralarge Virtual Screening Identifies SARS-CoV-2 Main Protease Inhibitors with Broad-Spectrum Activity against Coronaviruses.. <i>Journal of the American Chemical Society</i> , 2022 ,	16.4	16
60	Structure-Based Virtual Screening for Ligands of G Protein-Coupled Receptors: What Can Molecular Docking Do for You?. <i>Pharmacological Reviews</i> , 2021 , 73, 527-565	22.5	4
59	Fragment-based design of selective GPCR ligands guided by free energy simulations. <i>Chemical Communications</i> , 2021 , 57, 12305-12308	5.8	2
58	A practical guide to large-scale docking. <i>Nature Protocols</i> , 2021 , 16, 4799-4832	18.8	35
57	Can molecular dynamics simulations improve the structural accuracy and virtual screening performance of GPCR models?. <i>PLoS Computational Biology</i> , 2021 , 17, e1008936	5	2
56	Structure-Guided Design of G-Protein-Coupled Receptor Polypharmacology. <i>Angewandte Chemie</i> , 2021 , 133, 18170-18178	3.6	
55	Structure-Guided Design of G-Protein-Coupled Receptor Polypharmacology. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 18022-18030	16.4	6
54	Positive allosteric mechanisms of adenosine A receptor-mediated analgesia. <i>Nature</i> , 2021 , 597, 571-576	50.4	12
53	Identification of ligand-specific G protein-coupled receptor states and prediction of downstream efficacy via data-driven modeling. <i>ELife</i> , 2021 , 10,	8.9	5
52	Adenosine A receptor antagonists: from caffeine to selective non-xanthines. <i>British Journal of Pharmacology</i> , 2020 ,	8.6	19
51	The European Research Network on Signal Transduction (ERNEST): Toward a Multidimensional Holistic Understanding of G Protein-Coupled Receptor Signaling. <i>ACS Pharmacology and Translational Science</i> , 2020 , 3, 361-370	5.9	9
50	Performance of virtual screening against GPCR homology models: Impact of template selection and treatment of binding site plasticity. <i>PLoS Computational Biology</i> , 2020 , 16, e1007680	5	21
49	Docking Finds GPCR Ligands in Dark Chemical Matter. <i>Journal of Medicinal Chemistry</i> , 2020 , 63, 613-620	8.3	11
48	GPCRmd uncovers the dynamics of the 3D-GPCRome. <i>Nature Methods</i> , 2020 , 17, 777-787	21.6	34
47	Energy Landscapes Reveal Agonist Control of G Protein-Coupled Receptor Activation via Microswitches. <i>Biochemistry</i> , 2020 , 59, 880-891	3.2	16
46	Ligand design by targeting a binding site water. <i>Chemical Science</i> , 2020 , 12, 960-968	9.4	13
45	A conserved molecular switch in Class F receptors regulates receptor activation and pathway selection. <i>Nature Communications</i> , 2019 , 10, 667	17.4	35

44	Disruption of A2AR-D2R Heteroreceptor Complexes After A2AR Transmembrane 5 Peptide Administration Enhances Cocaine Self-Administration in Rats. <i>Molecular Neurobiology</i> , 2018 , 55, 7038-7048	6.2	34
43	Prediction of Ordered Water Molecules in Protein Binding Sites from Molecular Dynamics Simulations: The Impact of Ligand Binding on Hydration Networks. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 350-361	6.1	17
42	Scavenging of superoxide by a membrane-bound superoxide oxidase. <i>Nature Chemical Biology</i> , 2018 , 14, 788-793	11.7	32
41	FZD is a G-coupled receptor that exhibits the functional hallmarks of prototypical GPCRs. <i>Science Signaling</i> , 2018 , 11,	8.8	29
40	Structural Characterization of Agonist Binding to Protease-Activated Receptor 2 through Mutagenesis and Computational Modeling. <i>ACS Pharmacology and Translational Science</i> , 2018 , 1, 119-133	5.9	7
39	Mapping the Interface of a GPCR Dimer: A Structural Model of the A Adenosine and D Dopamine Receptor Heteromer. <i>Frontiers in Pharmacology</i> , 2018 , 9, 829	5.6	45
38	Docking Screens for Dual Inhibitors of Disparate Drug Targets for Parkinson's Disease. <i>Journal of Medicinal Chemistry</i> , 2018 , 61, 5269-5278	8.3	24
37	Structure-Based Discovery of GPCR Ligands from Crystal Structures and Homology Models. <i>Topics in Medicinal Chemistry</i> , 2017 , 65-99	0.4	1
36	Ligand Discovery for a Peptide-Binding GPCR by Structure-Based Screening of Fragment- and Lead-Like Chemical Libraries. <i>ACS Chemical Biology</i> , 2017 , 12, 735-745	4.9	19
35	Structure-Guided Screening for Functionally Selective D Dopamine Receptor Ligands from a Virtual Chemical Library. <i>ACS Chemical Biology</i> , 2017 , 12, 2652-2661	4.9	27
34	Fragment-Based Discovery and Optimization of Enzyme Inhibitors by Docking of Commercial Chemical Space. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 8160-8169	8.3	25
33	Agonist-induced dimer dissociation as a macromolecular step in G protein-coupled receptor signaling. <i>Nature Communications</i> , 2017 , 8, 226	17.4	45
32	Fragment optimization for GPCRs by molecular dynamics free energy calculations: Probing druggable subpockets of the A adenosine receptor binding site. <i>Scientific Reports</i> , 2017 , 7, 6398	4.9	28
31	The tyrosine Y250 in Frizzled 4 defines a conserved motif important for structural integrity of the receptor and recruitment of Disheveled. <i>Cellular Signalling</i> , 2017 , 38, 85-96	4.9	13
30	Understanding the Role of GPCR Heteroreceptor Complexes in Modulating the Brain Networks in Health and Disease. <i>Frontiers in Cellular Neuroscience</i> , 2017 , 11, 37	6.1	82
29	Structure-Based Screening of Uncharted Chemical Space for Atypical Adenosine Receptor Agonists. <i>ACS Chemical Biology</i> , 2016 , 11, 2763-2772	4.9	24
28	Fragment-Based Discovery of Subtype-Selective Adenosine Receptor Ligands from Homology Models. <i>Journal of Medicinal Chemistry</i> , 2015 , 58, 9578-90	8.3	19
27	Molecular docking screening using agonist-bound GPCR structures: probing the A2A adenosine receptor. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 550-63	6.1	55

26	Discovery of GPCR Ligands by Molecular Docking Screening: Novel Opportunities Provided by Crystal Structures. <i>Current Topics in Medicinal Chemistry</i> , 2015 , 15, 2484-503	3	29
25	Preferential activation by galanin 1-15 fragment of the GalR1 protomer of a GalR1-GalR2 heteroreceptor complex. <i>Biochemical and Biophysical Research Communications</i> , 2014 , 452, 347-53	3-4	32
24	Strategies for improved modeling of GPCR-drug complexes: blind predictions of serotonin receptors bound to ergotamine. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 2004-21	6.1	19
23	Structure-based discovery of selective serotonin 5-HT(1B) receptor ligands. <i>Structure</i> , 2014 , 22, 1140-1151	5.1	48
22	Insights into the role of Asp79(2.50) in α adrenergic receptor activation from molecular dynamics simulations. <i>Biochemistry</i> , 2014 , 53, 7283-96	3.2	40
21	Functional validation of virtual screening for novel agents with general anesthetic action at ligand-gated ion channels. <i>Molecular Pharmacology</i> , 2013 , 84, 670-8	4.3	16
20	Complementarity between in silico and biophysical screening approaches in fragment-based lead discovery against the A(2A) adenosine receptor. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 2701-14	6.1	55
19	Proton uptake and pKa changes in the uncoupled Asn139Cys variant of cytochrome c oxidase. <i>Biochemistry</i> , 2013 , 52, 827-36	3.2	13
18	Structure-based discovery of antagonists of nuclear receptor LRH-1. <i>Journal of Biological Chemistry</i> , 2013 , 288, 19830-44	5.4	68
17	Role of aspartate 132 at the orifice of a proton pathway in cytochrome c oxidase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 8912-7	11.5	19
16	Structure-activity relationships and molecular modeling of 1,2,4-triazoles as adenosine receptor antagonists. <i>ACS Medicinal Chemistry Letters</i> , 2012 , 3, 715-720	4.3	15
15	Ligand discovery from a dopamine D3 receptor homology model and crystal structure. <i>Nature Chemical Biology</i> , 2011 , 7, 769-78	11.7	250
14	Status of GPCR modeling and docking as reflected by community-wide GPCR Dock 2010 assessment. <i>Structure</i> , 2011 , 19, 1108-26	5.2	243
13	Structure-based discovery of A2A adenosine receptor ligands. <i>Journal of Medicinal Chemistry</i> , 2010 , 53, 3748-55	8.3	195
12	Charges for Large Scale Binding Free Energy Calculations with the Linear Interaction Energy Method. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 380-95	6.4	12
11	Absolute hydration entropies of alkali metal ions from molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 10255-60	3.4	36
10	Combining docking, molecular dynamics and the linear interaction energy method to predict binding modes and affinities for non-nucleoside inhibitors to HIV-1 reverse transcriptase. <i>Journal of Medicinal Chemistry</i> , 2008 , 51, 2648-56	8.3	75
9	Predicting binding modes from free energy calculations. <i>Journal of Medicinal Chemistry</i> , 2008 , 51, 2657-67	8.3	30

8	Active site of epoxide hydrolases revisited: a noncanonical residue in potato StEH1 promotes both formation and breakdown of the alkylenzyme intermediate. <i>Biochemistry</i> , 2007 , 46, 2466-79	3.2	19
7	Structures of Mycobacterium tuberculosis 1-deoxy-D-xylulose-5-phosphate reductoisomerase provide new insights into catalysis. <i>Journal of Biological Chemistry</i> , 2007 , 282, 19905-16	5.4	67
6	Improving the Accuracy of the Linear Interaction Energy Method for Solvation Free Energies. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 2162-75	6.4	97
5	Calculations of solute and solvent entropies from molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2006 , 8, 5385-95	3.6	62
4	Continuum solvation models in the linear interaction energy method. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 12034-41	3.4	47
3	Absolute and relative entropies from computer simulation with applications to ligand binding. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 6448-56	3.4	120
2	Proton binding to proteins: pK(a) calculations with explicit and implicit solvent models. <i>Journal of the American Chemical Society</i> , 2004 , 126, 4167-80	16.4	239
1	Energy landscapes reveal agonist control of GPCR activation via microswitches		4