Jens Carlsson

List of Publications by Citations

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	Ligand discovery from a dopamine D3 receptor homology model and crystal structure. *Nature Chemical Biology*, **2011**, 7, 769-78	11.7	250
60	Status of GPCR modeling and docking as reflected by community-wide GPCR Dock 2010 assessment. *Structure*, **2011**, 19, 1108-26	5.2	243
59	Proton binding to proteins: pK(a) calculations with explicit and implicit solvent models. *Journal of the American Chemical Society*, **2004**, 126, 4167-80	16.4	239
58	Structure-based discovery of A2A adenosine receptor ligands. *Journal of Medicinal Chemistry*, **2010**, 53, 3748-55	8.3	195
57	Absolute and relative entropies from computer simulation with applications to ligand binding. *Journal of Physical Chemistry B*, **2005**, 109, 6448-56	3.4	120
56	Improving the Accuracy of the Linear Interaction Energy Method for Solvation Free Energies. *Journal of Chemical Theory and Computation*, **2007**, 3, 2162-75	6.4	97
55	Understanding the Role of GPCR Heteroreceptor Complexes in Modulating the Brain Networks in Health and Disease. *Frontiers in Cellular Neuroscience*, **2017**, 11, 37	6.1	82
54	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. *Journal of Medicinal Chemistry*, **2008**, 51, 2648-56	8.3	75
53	Structure-based discovery of antagonists of nuclear receptor LRH-1. *Journal of Biological Chemistry*, **2013**, 288, 19830-44	5.4	68
52	Structures of Mycobacterium tuberculosis 1-deoxy-D-xylulose-5-phosphate reductoisomerase provide new insights into catalysis. *Journal of Biological Chemistry*, **2007**, 282, 19905-16	5.4	67
51	Calculations of solute and solvent entropies from molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2006**, 8, 5385-95	3.6	62
50	Complementarity between in silico and biophysical screening approaches in fragment-based lead discovery against the A(2A) adenosine receptor. *Journal of Chemical Information and Modeling*, **2013**, 53, 2701-14	6.1	55
49	Molecular docking screening using agonist-bound GPCR structures: probing the A2A adenosine receptor. *Journal of Chemical Information and Modeling*, **2015**, 55, 550-63	6.1	55
48	Structure-based discovery of selective serotonin 5-HT(1B) receptor ligands. *Structure*, **2014**, 22, 1140-1151	5.2	48
47	Continuum solvation models in the linear interaction energy method. *Journal of Physical Chemistry B*, **2006**, 110, 12034-41	3.4	47
46	Agonist-induced dimer dissociation as a macromolecular step in G protein-coupled receptor signaling. *Nature Communications*, **2017**, 8, 226	17.4	45
45	Mapping the Interface of a GPCR Dimer: A Structural Model of the A Adenosine and D Dopamine Receptor Heteromer. *Frontiers in Pharmacology*, **2018**, 9, 829	5.6	45

44	Insights into the role of Asp79(2.50) in β2 adrenergic receptor activation from molecular dynamics simulations. *Biochemistry*, **2014**, 53, 7283-96	3.2	40
43	Absolute hydration entropies of alkali metal ions from molecular dynamics simulations. *Journal of Physical Chemistry B*, **2009**, 113, 10255-60	3.4	36
42	A conserved molecular switch in Class F receptors regulates receptor activation and pathway selection. *Nature Communications*, **2019**, 10, 667	17.4	35
41	A practical guide to large-scale docking. *Nature Protocols*, **2021**, 16, 4799-4832	18.8	35
40	Disruption of A2AR-D2R Heteroreceptor Complexes After A2AR Transmembrane 5 Peptide Administration Enhances Cocaine Self-Administration in Rats. *Molecular Neurobiology*, **2018**, 55, 7038-7048	6.2	34
39	GPCRmd uncovers the dynamics of the 3D-GPCRome. *Nature Methods*, **2020**, 17, 777-787	21.6	34
38	Scavenging of superoxide by a membrane-bound superoxide oxidase. *Nature Chemical Biology*, **2018**, 14, 788-793	11.7	32
37	Preferential activation by galanin 1-15 fragment of the GalR1 protomer of a GalR1-GalR2 heteroreceptor complex. *Biochemical and Biophysical Research Communications*, **2014**, 452, 347-53	3.4	32
36	Predicting binding modes from free energy calculations. *Journal of Medicinal Chemistry*, **2008**, 51, 2657-67	8.3	30
35	Discovery of GPCR Ligands by Molecular Docking Screening: Novel Opportunities Provided by Crystal Structures. *Current Topics in Medicinal Chemistry*, **2015**, 15, 2484-503	3	29
34	FZD is a G-coupled receptor that exhibits the functional hallmarks of prototypical GPCRs. *Science Signaling*, **2018**, 11,	8.8	29
33	Fragment optimization for GPCRs by molecular dynamics free energy calculations: Probing druggable subpockets of the A adenosine receptor binding site. *Scientific Reports*, **2017**, 7, 6398	4.9	28
32	Structure-Guided Screening for Functionally Selective D Dopamine Receptor Ligands from a Virtual Chemical Library. *ACS Chemical Biology*, **2017**, 12, 2652-2661	4.9	27
31	Fragment-Based Discovery and Optimization of Enzyme Inhibitors by Docking of Commercial Chemical Space. *Journal of Medicinal Chemistry*, **2017**, 60, 8160-8169	8.3	25
30	Structure-Based Screening of Uncharted Chemical Space for Atypical Adenosine Receptor Agonists. *ACS Chemical Biology*, **2016**, 11, 2763-2772	4.9	24
29	Docking Screens for Dual Inhibitors of Disparate Drug Targets for Parkinson's Disease. *Journal of Medicinal Chemistry*, **2018**, 61, 5269-5278	8.3	24
28	Performance of virtual screening against GPCR homology models: Impact of template selection and treatment of binding site plasticity. *PLoS Computational Biology*, **2020**, 16, e1007680	5	21
27	Ligand Discovery for a Peptide-Binding GPCR by Structure-Based Screening of Fragment- and Lead-Like Chemical Libraries. *ACS Chemical Biology*, **2017**, 12, 735-745	4.9	19

26	Fragment-Based Discovery of Subtype-Selective Adenosine Receptor Ligands from Homology Models. *Journal of Medicinal Chemistry*, **2015**, 58, 9578-90	8.3	19
25	Adenosine A receptor antagonists: from caffeine to selective non-xanthines. *British Journal of Pharmacology*, **2020**,	8.6	19
24	Strategies for improved modeling of GPCR-drug complexes: blind predictions of serotonin receptors bound to ergotamine. *Journal of Chemical Information and Modeling*, **2014**, 54, 2004-21	6.1	19
23	Role of aspartate 132 at the orifice of a proton pathway in cytochrome c oxidase. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 8912-7	11.5	19
22	Active site of epoxide hydrolases revisited: a noncanonical residue in potato StEH1 promotes both formation and breakdown of the alkylenzyme intermediate. *Biochemistry*, **2007**, 46, 2466-79	3.2	19
21	Prediction of Ordered Water Molecules in Protein Binding Sites from Molecular Dynamics Simulations: The Impact of Ligand Binding on Hydration Networks. *Journal of Chemical Information and Modeling*, **2018**, 58, 350-361	6.1	17
20	Functional validation of virtual screening for novel agents with general anesthetic action at ligand-gated ion channels. *Molecular Pharmacology*, **2013**, 84, 670-8	4.3	16
19	Ultralarge Virtual Screening Identifies SARS-CoV-2 Main Protease Inhibitors with Broad-Spectrum Activity against Coronaviruses.. *Journal of the American Chemical Society*, **2022**,	16.4	16
18	Energy Landscapes Reveal Agonist Control of G Protein-Coupled Receptor Activation via Microswitches. *Biochemistry*, **2020**, 59, 880-891	3.2	16
17	Structure-activity relationships and molecular modeling of 1,2,4-triazoles as adenosine receptor antagonists. *ACS Medicinal Chemistry Letters*, **2012**, 3, 715-720	4.3	15
16	Proton uptake and pKa changes in the uncoupled Asn139Cys variant of cytochrome c oxidase. *Biochemistry*, **2013**, 52, 827-36	3.2	13
15	The tyrosine Y250 in Frizzled 4 defines a conserved motif important for structural integrity of the receptor and recruitment of Disheveled. *Cellular Signalling*, **2017**, 38, 85-96	4.9	13
14	Ligand design by targeting a binding site water. *Chemical Science*, **2020**, 12, 960-968	9.4	13
13	Charges for Large Scale Binding Free Energy Calculations with the Linear Interaction Energy Method. *Journal of Chemical Theory and Computation*, **2009**, 5, 380-95	6.4	12
12	Positive allosteric mechanisms of adenosine A receptor-mediated analgesia. *Nature*, **2021**, 597, 571-576	50.4	12
11	Docking Finds GPCR Ligands in Dark Chemical Matter. *Journal of Medicinal Chemistry*, **2020**, 63, 613-620	8.3	11
10	The European Research Network on Signal Transduction (ERNEST): Toward a Multidimensional Holistic Understanding of G Protein-Coupled Receptor Signaling. *ACS Pharmacology and Translational Science*, **2020**, 3, 361-370	5.9	9
9	Structural Characterization of Agonist Binding to Protease-Activated Receptor 2 through Mutagenesis and Computational Modeling. *ACS Pharmacology and Translational Science*, **2018**, 1, 119-133	5.9	7

List of Publications

8	Structure-Guided Design of G-Protein-Coupled Receptor Polypharmacology. *Angewandte Chemie - International Edition*, **2021**, 60, 18022-18030	16.4	6
7	Identification of ligand-specific G protein-coupled receptor states and prediction of downstream efficacy via data-driven modeling. *ELife*, **2021**, 10,	8.9	5
6	Structure-Based Virtual Screening for Ligands of G Protein-Coupled Receptors: What Can Molecular Docking Do for You?. *Pharmacological Reviews*, **2021**, 73, 527-565	22.5	4
5	Energy landscapes reveal agonist control of GPCR activation via microswitches		4
4	Fragment-based design of selective GPCR ligands guided by free energy simulations. *Chemical Communications*, **2021**, 57, 12305-12308	5.8	2
3	Can molecular dynamics simulations improve the structural accuracy and virtual screening performance of GPCR models?. *PLoS Computational Biology*, **2021**, 17, e1008936	5	2
2	Structure-Based Discovery of GPCR Ligands from Crystal Structures and Homology Models. *Topics in Medicinal Chemistry*, **2017**, 65-99	0.4	1
1	Structure-Guided Design of G-Protein-Coupled Receptor Polypharmacology. *Angewandte Chemie*, **2021**, 133, 18170-18178	3.6	