Jens Carlsson

List of Publications by Year
in descending order

61 papers	3,741 citations	136950 32 h-index	138484 58 g-index
66 all docs	66 docs citations	66 times ranked	4238 citing authors

#	Article	IF	Citations
1	Ligand discovery from a dopamine D3 receptor homology model and crystal structure. Nature Chemical Biology, 2011, 7, 769-778.	8.0	285
2	Status of GPCR Modeling and Docking as Reflected by Community-wide GPCR Dock 2010 Assessment. Structure, 2011, 19, 1108-1126.	3.3	269
3	Proton Binding to Proteins:Â pKaCalculations with Explicit and Implicit Solvent Models. Journal of the American Chemical Society, 2004, 126, 4167-4180.	13.7	266
4	Structure-Based Discovery of A_{2A}Adenosine Receptor Ligands. Journal of Medicinal Chemistry, 2010, 53, 3748-3755.	6.4	212
5	A practical guide to large-scale docking. Nature Protocols, 2021, 16, 4799-4832.	12.0	206
6	Absolute and Relative Entropies from Computer Simulation with Applications to Ligand Binding. Journal of Physical Chemistry B, 2005, 109, 6448-6456.	2.6	130
7	Ultralarge Virtual Screening Identifies SARS-CoV-2 Main Protease Inhibitors with Broad-Spectrum Activity against Coronaviruses. Journal of the American Chemical Society, 2022, 144, 2905-2920.	13.7	118
8	Improving the Accuracy of the Linear Interaction Energy Method for Solvation Free Energies. Journal of Chemical Theory and Computation, 2007, 3, 2162-2175.	5.3	112
9	Understanding the Role of GPCR Heteroreceptor Complexes in Modulating the Brain Networks in Health and Disease. Frontiers in Cellular Neuroscience, 2017, 11, 37.	3.7	110
10	GPCRmd uncovers the dynamics of the 3D-GPCRome. Nature Methods, 2020, 17, 777-787.	19.0	90
11	Structure-based Discovery of Antagonists of Nuclear Receptor LRH-1. Journal of Biological Chemistry, 2013, 288, 19830-19844.	3.4	89
12	Positive allosteric mechanisms of adenosine A1 receptor-mediated analgesia. Nature, 2021, 597, 571-576.	27.8	84
13	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, 2648-2656.	6.4	79
14	Structures of Mycobacterium tuberculosis 1-Deoxy-D-xylulose-5-phosphate Reductoisomerase Provide New Insights into Catalysis. Journal of Biological Chemistry, 2007, 282, 19905-19916.	3.4	77
15	Scavenging of superoxide by a membrane-bound superoxide oxidase. Nature Chemical Biology, 2018, 14, 788-793.	8.0	71
16	Calculations of solute and solvent entropies from molecular dynamics simulations. Physical Chemistry Chemical Physics, 2006, 8, 5385-5395.	2.8	69
17	Insights into the Role of Asp79^{2.50} in Î²₂ Adrenergic Receptor Activation from Molecular Dynamics Simulations. Biochemistry, 2014, 53, 7283-7296.	2.5	67
18	Complementarity between in Silico and Biophysical Screening Approaches in Fragment-Based Lead Discovery against the A2A Adenosine Receptor. Journal of Chemical Information and Modeling, 2013, 53, 2701-2714.	5.4	65

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19	Molecular Docking Screening Using Agonist-Bound GPCR Structures: Probing the A_{2A} Adenosine Receptor. Journal of Chemical Information and Modeling, 2015, 55, 550-563.	5.4	65
20	Mapping the Interface of a GPCR Dimer: A Structural Model of the A2A Adenosine and D2 Dopamine Receptor Heteromer. Frontiers in Pharmacology, 2018, 9, 829.	3.5	62
21	Structure-Based Virtual Screening for Ligands of G Proteinâ€"Coupled Receptors: What Can Molecular Docking Do for You?. Pharmacological Reviews, 2021, 73, 1698-1736.	16.0	61
22	Structure-Based Discovery of Selective Serotonin 5-HT 1B Receptor Ligands. Structure, 2014, 22, 1140-1151.	3.3	57
23	Agonist-induced dimer dissociation as a macromolecular step in G protein-coupled receptor signaling. Nature Communications, 2017, 8, 226.	12.8	57
24	A conserved molecular switch in Class F receptors regulates receptor activation and pathway selection. Nature Communications, 2019, 10, 667.	12.8	56
25	Continuum Solvation Models in the Linear Interaction Energy Method. Journal of Physical Chemistry B, 2006, 110, 12034-12041.	2.6	52
26	Adenosine A_{2A} receptor antagonists: from caffeine to selective nonâ€xanthines. British Journal of Pharmacology, 2022, 179, 3496-3511.	5.4	48
27	FZD ₅ is a GÎ± _q -coupled receptor that exhibits the functional hallmarks of prototypical GPCRs. Science Signaling, 2018, 11, .	3.6	46
28	Energy Landscapes Reveal Agonist Control of G Protein-Coupled Receptor Activation via Microswitches. Biochemistry, 2020, 59, 880-891.	2.5	45
29	Fragment optimization for GPCRs by molecular dynamics free energy calculations: Probing druggable subpockets of the A 2A adenosine receptor binding site. Scientific Reports, 2017, 7, 6398.	3.3	44
30	Disruption of A2AR-D2R Heteroreceptor Complexes After A2AR Transmembrane 5 Peptide Administration Enhances Cocaine Self-Administration in Rats. Molecular Neurobiology, 2018, 55, 7038-7048.	4.0	43
31	Absolute Hydration Entropies of Alkali Metal Ions from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 10255-10260.	2.6	41
32	Docking Screens for Dual Inhibitors of Disparate Drug Targets for Parkinsonâ€™s Disease. Journal of Medicinal Chemistry, 2018, 61, 5269-5278.	6.4	40
33	Identification of ligand-specific G protein-coupled receptor states and prediction of downstream efficacy via data-driven modeling. ELife, 2021, 10, .	6.0	40
34	Preferential activation by galanin 1â€"15 fragment of the GalR1 protomer of a GalR1â€"GalR2 heteroreceptor complex. Biochemical and Biophysical Research Communications, 2014, 452, 347-353.	2.1	38
35	Performance of virtual screening against GPCR homology models: Impact of template selection and treatment of binding site plasticity. PLoS Computational Biology, 2020, 16, e1007680.	3.2	35
36	Predicting Binding Modes from Free Energy Calculations. Journal of Medicinal Chemistry, 2008, 51, 2657-2667.	6.4	34

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37	Ligand design by targeting a binding site water. Chemical Science, 2021, 12, 960-968.	7.4	34
38	Structure-Guided Screening for Functionally Selective D₂ Dopamine Receptor Ligands from a Virtual Chemical Library. ACS Chemical Biology, 2017, 12, 2652-2661.	3.4	32
39	Fragment-Based Discovery and Optimization of Enzyme Inhibitors by Docking of Commercial Chemical Space. Journal of Medicinal Chemistry, 2017, 60, 8160-8169.	6.4	32
40	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.	5.4	32
41	Discovery of GPCR Ligands by Molecular Docking Screening: Novel Opportunities Provided by Crystal Structures. Current Topics in Medicinal Chemistry, 2015, 15, 2484-2503.	2.1	31
42	Structure-Based Screening of Uncharted Chemical Space for Atypical Adenosine Receptor Agonists. ACS Chemical Biology, 2016, 11, 2763-2772.	3.4	28
43	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.	3.4	24
44	Fragment-Based Discovery of Subtype-Selective Adenosine Receptor Ligands from Homology Models. Journal of Medicinal Chemistry, 2015, 58, 9578-9590.	6.4	23
45	Strategies for Improved Modeling of GPCR-Drug Complexes: Blind Predictions of Serotonin Receptors Bound to Ergotamine. Journal of Chemical Information and Modeling, 2014, 54, 2004-2021.	5.4	21
46	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, 8912-8917.	7.1	20
47	Active Site of Epoxide Hydrolases Revisited:â€‰ A Noncanonical Residue in Potato StEH1 Promotes both Formation and Breakdown of the Alkylenzyme Intermediate. Biochemistry, 2007, 46, 2466-2479.	2.5	19
48	Functional Validation of Virtual Screening for Novel Agents with General Anesthetic Action at Ligand-Gated Ion Channels. Molecular Pharmacology, 2013, 84, 670-678.	2.3	19
49	Structureâ€“Activity Relationships and Molecular Modeling of 1,2,4-Triazoles as Adenosine Receptor Antagonists. ACS Medicinal Chemistry Letters, 2012, 3, 715-720.	2.8	17
50	The tyrosine Y2502.39 in Frizzled 4 defines a conserved motif important for structural integrity of the receptor and recruitment of Disheveled. Cellular Signalling, 2017, 38, 85-96.	3.6	16
51	Can molecular dynamics simulations improve the structural accuracy and virtual screening performance of GPCR models?. PLoS Computational Biology, 2021, 17, e1008936.	3.2	16
52	Proton Uptake and pKa Changes in the Uncoupled Asn139Cys Variant of Cytochrome c Oxidase. Biochemistry, 2013, 52, 827-836.	2.5	15
53	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.	4.9	15
54	Importance of Binding Site Hydration and Flexibility Revealed When Optimizing a Macrocyclic Inhibitor of the Keap1â€“Nrf2 Proteinâ€“Protein Interaction. Journal of Medicinal Chemistry, 2022, 65, 3473-3517.	6.4	14

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55	Docking Finds GPCR Ligands in Dark Chemical Matter. Journal of Medicinal Chemistry, 2020, 63, 613-620.	6.4	13
56	Charges for Large Scale Binding Free Energy Calculations with the Linear Interaction Energy Method. Journal of Chemical Theory and Computation, 2009, 5, 380-395.	5.3	12
57	Structureâ€Guided Design of Gâ€Proteinâ€Coupled Receptor Polypharmacology. Angewandte Chemie - International Edition, 2021, 60, 18022-18030.	13.8	12
58	Fragment-based design of selective GPCR ligands guided by free energy simulations. Chemical Communications, 2021, 57, 12305-12308.	4.1	11
59	Structural Characterization of Agonist Binding to Protease-Activated Receptor 2 through Mutagenesis and Computational Modeling. ACS Pharmacology and Translational Science, 2018, 1, 119-133.	4.9	9
60	Structure-Based Discovery of GPCR Ligands from Crystal Structures and Homology Models. Topics in Medicinal Chemistry, 2017, , 65-99.	0.8	3
61	Structureâ€Guided Design of Gâ€Proteinâ€Coupled Receptor Polypharmacology. Angewandte Chemie, 2021, 133, 18170-18178.	2.0	0