

Ravinder Abrol

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69
papers

1,694
citations

26
h-index

39
g-index

83
ext. papers

1,888
ext. citations

4.8
avg, IF

4.49
L-index

#	Paper	IF	Citations
69	Low-frequency and rare exome chip variants associate with fasting glucose and type 2 diabetes susceptibility. <i>Nature Communications</i> , 2015 , 6, 5897	17.4	147
68	FOXC1 Activates Smoothed-Independent Hedgehog Signaling in Basal-like Breast Cancer. <i>Cell Reports</i> , 2015 , 13, 1046-58	10.6	94
67	Elucidating glycosaminoglycan-protein-protein interactions using carbohydrate microarray and computational approaches. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011 , 108, 9747-52	11.5	82
66	An optimal adiabatic-to-diabatic transformation of the 1 2A? and 2 2A? states of H3. <i>Journal of Chemical Physics</i> , 2002 , 116, 1035-1062	3.9	81
65	Predictions of CCR1 chemokine receptor structure and BX 471 antagonist binding followed by experimental validation. <i>Journal of Biological Chemistry</i> , 2006 , 281, 27613-20	5.4	78
64	Genetically encoded photo-cross-linkers map the binding site of an allosteric drug on a G protein-coupled receptor. <i>ACS Chemical Biology</i> , 2012 , 7, 967-72	4.9	59
63	Accurate first-derivative nonadiabatic couplings for the H3 system. <i>Journal of Chemical Physics</i> , 2001 , 115, 4640-4659	3.9	59
62	3D structure prediction of TAS2R38 bitter receptors bound to agonists phenylthiocarbamide (PTC) and 6-n-propylthiouracil (PROP). <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 1875-85	6.1	56
61	Structure-Based Sequence Alignment of the Transmembrane Domains of All Human GPCRs: Phylogenetic, Structural and Functional Implications. <i>PLoS Computational Biology</i> , 2016 , 12, e1004805	5	56
60	The glove-like structure of the conserved membrane protein TatC provides insight into signal sequence recognition in twin-arginine translocation. <i>Structure</i> , 2013 , 21, 777-88	5.2	49
59	Predicted 3D structures for adenosine receptors bound to ligands: comparison to the crystal structure. <i>Journal of Structural Biology</i> , 2010 , 170, 10-20	3.4	48
58	Antifreeze proteins govern the precipitation of trehalose in a freezing-avoiding insect at low temperature. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 6683-8	11.5	42
57	Predicted structure of agonist-bound glucagon-like peptide 1 receptor, a class B G protein-coupled receptor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 19988-93	11.5	41
56	Activation mechanism of the G protein-coupled sweet receptor heterodimer with sweeteners and allosteric agonists. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 2568-2573	11.5	39
55	Bihelix: Towards de novo structure prediction of an ensemble of G-protein coupled receptor conformations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012 , 80, 505-18	4.2	37
54	Structure-based prediction of subtype selectivity of histamine H3 receptor selective antagonists in clinical trials. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 3262-74	6.1	36
53	Identification and characterization of an activating F229V substitution in the V2 vasopressin receptor in an infant with NSIAD. <i>Journal of the American Society of Nephrology: JASN</i> , 2012 , 23, 1635-40 ^{12.7}	12.7	36

52	3-Dimensional structures of G protein-coupled receptors and binding sites of agonists and antagonists. <i>Journal of Nutrition</i> , 2007 , 137, 1528S-1538S; discussion 1548S	4.1	34
51	Molecular basis for dramatic changes in cannabinoid CB1 G protein-coupled receptor activation upon single and double point mutations. <i>Protein Science</i> , 2013 , 22, 101-13	6.3	33
50	Biological chiral recognition: the substrate's perspective. <i>Chirality</i> , 2005 , 17 Suppl, S30-9	2.1	32
49	Computationally-predicted CB1 cannabinoid receptor mutants show distinct patterns of salt-bridges that correlate with their level of constitutive activity reflected in G protein coupling levels, thermal stability, and ligand binding. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013 , 81, 1304-17	4.2	30
48	Rottlerin stimulates apoptosis in pancreatic cancer cells through interactions with proteins of the Bcl-2 family. <i>American Journal of Physiology - Renal Physiology</i> , 2010 , 298, G63-73	5.1	30
47	Use of G-protein-coupled and -uncoupled CCR5 receptors by CCR5 inhibitor-resistant and -sensitive human immunodeficiency virus type 1 variants. <i>Journal of Virology</i> , 2013 , 87, 6569-81	6.6	29
46	Ligand- and mutation-induced conformational selection in the CCR5 chemokine G protein-coupled receptor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, 13040-5	11.5	28
45	Predicted structures of agonist and antagonist bound complexes of adenosine A3 receptor. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011 , 79, 1878-97	4.2	27
44	Experimental validation of the predicted binding site of Escherichia coli K1 outer membrane protein A to human brain microvascular endothelial cells: identification of critical mutations that prevent E. coli meningitis. <i>Journal of Biological Chemistry</i> , 2010 , 285, 37753-61	5.4	27
43	A bitter pill for type 2 diabetes? The activation of bitter taste receptor TAS2R38 can stimulate GLP-1 release from enteroendocrine L-cells. <i>Biochemical and Biophysical Research Communications</i> , 2016 , 475, 295-300	3.4	26
42	Towards a general model for protein-substrate stereoselectivity. <i>Protein Science</i> , 2002 , 11, 1330-9	6.3	26
41	SuperBiHelix method for predicting the pleiotropic ensemble of G-protein-coupled receptor conformations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, E72-8	11.5	25
40	Predicted structures and dynamics for agonists and antagonists bound to serotonin 5-HT2B and 5-HT2C receptors. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 420-33	6.1	25
39	Structure prediction of G protein-coupled receptors and their ensemble of functionally important conformations. <i>Methods in Molecular Biology</i> , 2012 , 914, 237-54	1.4	22
38	Nonadiabatic effects in the H + H2 exchange reaction: accurate quantum dynamics calculations at a state-to-state level. <i>Journal of Chemical Physics</i> , 2009 , 130, 144301	3.9	22
37	Novel purine-based fluoroaryl-1,2,3-triazoles as neuroprotecting agents: synthesis, neuronal cell culture investigations, and CDK5 docking studies. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2011 , 21, 3957-61	2.9	21
36	Quantum Reaction Dynamics for Multiple Electronic States. <i>Advances in Chemical Physics</i> , 2003 , 283-322		20
35	Predicting glycosaminoglycan surface protein interactions and implications for studying axonal growth. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 13697-13702	11.5	19

34	Prediction of the three-dimensional structure for the rat urotensin II receptor, and comparison of the antagonist binding sites and binding selectivity between human and rat receptors from atomistic simulations. <i>ChemMedChem</i> , 2010 , 5, 1594-608	3.7	18
33	Geometric phase effects in H3 predissociation. <i>Physical Review A</i> , 2007 , 76,	2.6	17
32	Characterizing and predicting the functional and conformational diversity of seven-transmembrane proteins. <i>Methods</i> , 2011 , 55, 405-14	4.6	15
31	Ethanol Induced Disordering of Pancreatic Acinar Cell Endoplasmic Reticulum: An ER Stress/Defective Unfolded Protein Response Model. <i>Cellular and Molecular Gastroenterology and Hepatology</i> , 2018 , 5, 479-497	7.9	14
30	Conformational ensemble view of G protein-coupled receptors and the effect of mutations and ligand binding. <i>Methods in Enzymology</i> , 2013 , 520, 31-48	1.7	14
29	The interaction of N-glycans in Fcγ receptor I β chain with Escherichia coli K1 outer membrane protein A for entry into macrophages: experimental and computational analysis. <i>Journal of Biological Chemistry</i> , 2014 , 289, 30937-49	5.4	12
28	A quantum and semiclassical study of dynamical resonances in the C+NO- \rightarrow CO reaction. <i>Journal of Chemical Physics</i> , 2001 , 114, 7461-7470	3.9	10
27	Down-regulation of pancreatic and duodenal homeobox-1 by somatostatin receptor subtype 5: a novel mechanism for inhibition of cellular proliferation and insulin secretion by somatostatin. <i>Frontiers in Physiology</i> , 2014 , 5, 226	4.6	8
26	Conformational and Thermodynamic Landscape of GPCR Activation from Theory and Computation. <i>Biophysical Journal</i> , 2016 , 110, 2618-2629	2.9	7
25	The 3D Structure of Human DP Prostaglandin G-Protein-Coupled Receptor Bound to Cyclopentanoindole Antagonist, Predicted Using the DuplexBiHelix Modification of the GEnSeMBLE Method. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 1624-1642	6.4	6
24	1,3-Sigmatropic fluorine migration to boron in McLafferty type of rearrangements: Observation of tetrafluorobenzene radical cation and trifluorobenzene cation by CID-mass spectrometry. <i>Journal of Organometallic Chemistry</i> , 2013 , 747, 133-139	2.3	6
23	HER3-targeted protein chimera forms endosomolytic capsomeres and self-assembles into stealth nucleocapsids for systemic tumor homing of RNA interference in vivo. <i>Nucleic Acids Research</i> , 2019 , 47, 11020-11043	20.1	5
22	The predicted ensemble of low-energy conformations of human somatostatin receptor subtype 5 and the binding of antagonists. <i>ChemMedChem</i> , 2015 , 10, 650-61	3.7	5
21	Structural basis for bitter taste receptor activation and its potential role in targeting diabetes. <i>Functional Foods in Health and Disease</i> , 2015 , 5, 117	2.5	5
20	Resistance to receptor-blocking therapies primes tumors as targets for HER3-homing nanobiologics. <i>Journal of Controlled Release</i> , 2018 , 271, 127-138	11.7	4
19	Computational Prediction and Biochemical Analyses of New Inverse Agonists for the CB1 Receptor. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 201-12	6.1	4
18	Understanding G Protein Selectivity of Muscarinic Acetylcholine Receptors Using Computational Methods. <i>International Journal of Molecular Sciences</i> , 2019 , 20,	6.3	4
17	The Predicted 3D Structure of Bitter Taste Receptors, TAS2R38 Based on a BiHelix and SuperBiHelix Methodologies. <i>Procedia Environmental Sciences</i> , 2011 , 8, 543-548		4

16	Pseudo-Symmetric Assembly of Protodomains as a Common Denominator in the Evolution of Polytropic Helical Membrane Proteins. <i>Journal of Molecular Evolution</i> , 2020 , 88, 319-344	3.1	3
15	Identifying multiple active conformations in the G protein-coupled receptor activation landscape using computational methods. <i>Methods in Cell Biology</i> , 2017 , 142, 173-186	1.8	3
14	Chapter 11:G Protein-Coupled Receptors: Conformational Gatekeepers of Transmembrane Signal Transduction and Diversification. <i>RSC Drug Discovery Series</i> , 2011 , 188-229	0.6	3
13	The complex role of the N-terminus and acidic residues of HdeA as pH-dependent switches in its chaperone function. <i>Biophysical Chemistry</i> , 2020 , 264, 106406	3.5	3
12	A beetle antifreeze protein protects lactate dehydrogenase under freeze-thawing. <i>International Journal of Biological Macromolecules</i> , 2019 , 136, 1153-1160	7.9	2
11	Molecular basis for the interplay of apoptosis and proliferation mediated by Bcl-xL:Bim interactions in pancreatic cancer cells. <i>Biochemical and Biophysical Research Communications</i> , 2012 , 422, 596-601	3.4	1
10	Reduced potential energy curves for diatomic molecules and their respective cations. <i>Chemical Physics Letters</i> , 1999 , 312, 341-345	2.5	1
9	7-Transmembrane Helical (7TMH) Proteins: Pseudo-Symmetry and Conformational Plasticity		1
8	Chiral Graphs: Reduced Representations of Ligand Scaffolds for Stereoselective Biomolecular Recognition, Drug Design, and Enhanced Exploration of Chemical Structure Space. <i>ChemMedChem</i> , 2019 , 14, 798-809	3.7	1
7	Development of enhanced conformational sampling methods to probe the activation landscape of GPCRs. <i>Advances in Protein Chemistry and Structural Biology</i> , 2022 , 128, 325-359	5.3	0
6	Computation of Vapor Pressure. <i>Journal of Chemical Education</i> , 1995 , 72, 1083	2.4	
5	A Structural Framework for the G Protein Selectivity of Muscarinic Acetylcholine GPCRs. <i>FASEB Journal</i> , 2020 , 34, 1-1	0.9	
4	Unbiased topological parameters to characterize the signatures of GPCR conformational changes. <i>FASEB Journal</i> , 2020 , 34, 1-1	0.9	
3	Mechanisms of G Protein-Selectivity in Muscarinic Acetylcholine Receptor Family. <i>FASEB Journal</i> , 2019 , 33, 779.35	0.9	
2	Understanding G Protein Selectivity of Dopamine Receptors Using Computational Methods. <i>FASEB Journal</i> , 2019 , 33, 477.9	0.9	
1	Development of New Methods for Enhanced Conformational Sampling of GPCRs. <i>FASEB Journal</i> , 2020 , 34, 1-1	0.9	