Ravinder Abrol

List of Publications by Year in Descending Order

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	Development of enhanced conformational sampling methods to probe the activation landscape of GPCRs.. *Advances in Protein Chemistry and Structural Biology*, **2022**, 128, 325-359	5.3	0
68	Pseudo-Symmetric Assembly of Protodomains as a Common Denominator in the Evolution of Polytopic Helical Membrane Proteins. *Journal of Molecular Evolution*, **2020**, 88, 319-344	3.1	3
67	A Structural Framework for the G Protein Selectivity of Muscarinic Acetylcholine GPCRs. *FASEB Journal*, **2020**, 34, 1-1	0.9	
66	Unbiased topological parameters to characterize the signatures of GPCR conformational changes. *FASEB Journal*, **2020**, 34, 1-1	0.9	
65	Development of New Methods for Enhanced Conformational Sampling of GPCRs. *FASEB Journal*, **2020**, 34, 1-1	0.9	
64	The complex role of the N-terminus and acidic residues of HdeA as pH-dependent switches in its chaperone function. *Biophysical Chemistry*, **2020**, 264, 106406	3.5	3
63	A beetle antifreeze protein protects lactate dehydrogenase under freeze-thawing. *International Journal of Biological Macromolecules*, **2019**, 136, 1153-1160	7.9	2
62	HER3-targeted protein chimera forms endosomolytic capsomeres and self-assembles into stealth nucleocapsids for systemic tumor homing of RNA interference in vivo. *Nucleic Acids Research*, **2019**, 47, 11020-11043	20.1	5
61	Understanding G Protein Selectivity of Muscarinic Acetylcholine Receptors Using Computational Methods. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	4
60	Mechanisms of G Protein-Selectivity in Muscarinic Acetylcholine Receptor Family. *FASEB Journal*, **2019**, 33, 779.35	0.9	
59	Understanding G Protein Selectivity of Dopamine Receptors Using Computational Methods. *FASEB Journal*, **2019**, 33, 477.9	0.9	
58	Chiral Graphs: Reduced Representations of Ligand Scaffolds for Stereoselective Biomolecular Recognition, Drug Design, and Enhanced Exploration of Chemical Structure Space. *ChemMedChem*, **2019**, 14, 798-809	3.7	1
57	The 3D Structure of Human DP Prostaglandin G-Protein-Coupled Receptor Bound to Cyclopentanoindole Antagonist, Predicted Using the DuplexBiHelix Modification of the GEnSeMBLE Method. *Journal of Chemical Theory and Computation*, **2018**, 14, 1624-1642	6.4	6
56	Resistance to receptor-blocking therapies primes tumors as targets for HER3-homing nanobiologics. *Journal of Controlled Release*, **2018**, 271, 127-138	11.7	4
55	Ethanol Induced Disordering of Pancreatic Acinar Cell Endoplasmic Reticulum: An ER Stress/Defective Unfolded Protein Response Model. *Cellular and Molecular Gastroenterology and Hepatology*, **2018**, 5, 479-497	7.9	14
54	Activation mechanism of the G protein-coupled sweet receptor heterodimer with sweeteners and allosteric agonists. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 2568-2573	11.5	39
53	Predicting glycosaminoglycan surface protein interactions and implications for studying axonal growth. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 13697-13702	11.5	19

52	Identifying multiple active conformations in the G protein-coupled receptor activation landscape using computational methods. *Methods in Cell Biology*, **2017**, 142, 173-186	1.8	3
51	Conformational and Thermodynamic Landscape of GPCR Activation from Theory and Computation. *Biophysical Journal*, **2016**, 110, 2618-2629	2.9	7
50	A bitter pill for type 2 diabetes? The activation of bitter taste receptor TAS2R38 can stimulate GLP-1 release from enteroendocrine L-cells. *Biochemical and Biophysical Research Communications*, **2016**, 475, 295-300	3.4	26
49	Computational Prediction and Biochemical Analyses of New Inverse Agonists for the CB1 Receptor. *Journal of Chemical Information and Modeling*, **2016**, 56, 201-12	6.1	4
48	Structure-Based Sequence Alignment of the Transmembrane Domains of All Human GPCRs: Phylogenetic, Structural and Functional Implications. *PLoS Computational Biology*, **2016**, 12, e1004805	5	56
47	Antifreeze proteins govern the precipitation of trehalose in a freezing-avoiding insect at low temperature. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 6683-8	11.5	42
46	FOXC1 Activates Smoothened-Independent Hedgehog Signaling in Basal-like Breast Cancer. *Cell Reports*, **2015**, 13, 1046-58	10.6	94
45	The predicted ensemble of low-energy conformations of human somatostatin receptor subtype 5 and the binding of antagonists. *ChemMedChem*, **2015**, 10, 650-61	3.7	5
44	Low-frequency and rare exome chip variants associate with fasting glucose and type 2 diabetes susceptibility. *Nature Communications*, **2015**, 6, 5897	17.4	147
43	Structural basis for bitter taste receptor activation and its potential role in targeting diabetes. *Functional Foods in Health and Disease*, **2015**, 5, 117	2.5	5
42	SuperBiHelix method for predicting the pleiotropic ensemble of G-protein-coupled receptor conformations. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, E72-8	11.5	25
41	Ligand- and mutation-induced conformational selection in the CCR5 chemokine G protein-coupled receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 13040-5	11.5	28
40	The interaction of N-glycans in Fc□receptor I E□chain with Escherichia coli K1 outer membrane protein A for entry into macrophages: experimental and computational analysis. *Journal of Biological Chemistry*, **2014**, 289, 30937-49	5.4	12
39	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. *Frontiers in Physiology*, **2014**, 5, 226	4.6	8
38	Conformational ensemble view of G protein-coupled receptors and the effect of mutations and ligand binding. *Methods in Enzymology*, **2013**, 520, 31-48	1.7	14
37	Molecular basis for dramatic changes in cannabinoid CB1 G protein-coupled receptor activation upon single and double point mutations. *Protein Science*, **2013**, 22, 101-13	6.3	33
36	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. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 1304-17	4.2	30
35	The glove-like structure of the conserved membrane protein TatC provides insight into signal sequence recognition in twin-arginine translocation. *Structure*, **2013**, 21, 777-88	5.2	49

34	1,3-Sigmatropic fluorine migration to boron in McLafferty type of rearrangements: Observation of tetrafluorobenzyne radical cation and trifluorobenzyne cation by CID-mass spectrometry. *Journal of Organometallic Chemistry*, **2013**, 747, 133-139	2.3	6
33	Use of G-protein-coupled and -uncoupled CCR5 receptors by CCR5 inhibitor-resistant and -sensitive human immunodeficiency virus type 1 variants. *Journal of Virology*, **2013**, 87, 6569-81	6.6	29
32	Predicted structure of agonist-bound glucagon-like peptide 1 receptor, a class B G protein-coupled receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 19988-93	11.5	41
31	Genetically encoded photo-cross-linkers map the binding site of an allosteric drug on a G protein-coupled receptor. *ACS Chemical Biology*, **2012**, 7, 967-72	4.9	59
30	Structure prediction of G protein-coupled receptors and their ensemble of functionally important conformations. *Methods in Molecular Biology*, **2012**, 914, 237-54	1.4	22
29	Molecular basis for the interplay of apoptosis and proliferation mediated by Bcl-xL:Bim interactions in pancreatic cancer cells. *Biochemical and Biophysical Research Communications*, **2012**, 422, 596-601	3.4	1
28	3D structure prediction of TAS2R38 bitter receptors bound to agonists phenylthiocarbamide (PTC) and 6-n-propylthiouracil (PROP). *Journal of Chemical Information and Modeling*, **2012**, 52, 1875-85	6.1	56
27	Bihelix: Towards de novo structure prediction of an ensemble of G-protein coupled receptor conformations. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 505-18	4.2	37
26	Identification and characterization of an activating F229V substitution in the V2 vasopressin receptor in an infant with NSIAD. *Journal of the American Society of Nephrology: JASN*, **2012**, 23, 1635-40	12.7	36
25	Structure-based prediction of subtype selectivity of histamine H3 receptor selective antagonists in clinical trials. *Journal of Chemical Information and Modeling*, **2011**, 51, 3262-74	6.1	36
24	Characterizing and predicting the functional and conformational diversity of seven-transmembrane proteins. *Methods*, **2011**, 55, 405-14	4.6	15
23	The Predicted 3D Structure of Bitter Taste Receptors, TAS2R38 Based on a BiHelix and SuperBiHelix Methodologies. *Procedia Environmental Sciences*, **2011**, 8, 543-548		4
22	Predicted structures and dynamics for agonists and antagonists bound to serotonin 5-HT2B and 5-HT2C receptors. *Journal of Chemical Information and Modeling*, **2011**, 51, 420-33	6.1	25
21	Predicted structures of agonist and antagonist bound complexes of adenosine A3 receptor. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 1878-97	4.2	27
20	Novel purine-based fluoroaryl-1,2,3-triazoles as neuroprotecting agents: synthesis, neuronal cell culture investigations, and CDK5 docking studies. *Bioorganic and Medicinal Chemistry Letters*, **2011**, 21, 3957-61	2.9	21
19	Elucidating glycosaminoglycan-protein-protein interactions using carbohydrate microarray and computational approaches. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 9747-52	11.5	82
18	Chapter 11:G Protein-Coupled Receptors: Conformational Gatekeepers of Transmembrane Signal Transduction and Diversification. *RSC Drug Discovery Series*, **2011**, 188-229	0.6	3
17	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. *Journal of Biological Chemistry*, **2010**, 285, 37753-61	5.4	27

16	Predicted 3D structures for adenosine receptors bound to ligands: comparison to the crystal structure. *Journal of Structural Biology*, **2010**, 170, 10-20	3.4	48
15	Rottlerin stimulates apoptosis in pancreatic cancer cells through interactions with proteins of the Bcl-2 family. *American Journal of Physiology - Renal Physiology*, **2010**, 298, G63-73	5.1	30
14	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. *ChemMedChem*, **2010**, 5, 1594-608	3.7	18
13	Nonadiabatic effects in the H + H2 exchange reaction: accurate quantum dynamics calculations at a state-to-state level. *Journal of Chemical Physics*, **2009**, 130, 144301	3.9	22
12	3-Dimensional structures of G protein-coupled receptors and binding sites of agonists and antagonists. *Journal of Nutrition*, **2007**, 137, 1528S-1538S; discussion 1548S	4.1	34
11	Geometric phase effects in H3 predissociation. *Physical Review A*, **2007**, 76,	2.6	17
10	Predictions of CCR1 chemokine receptor structure and BX 471 antagonist binding followed by experimental validation. *Journal of Biological Chemistry*, **2006**, 281, 27613-20	5.4	78
9	Biological chiral recognition: the substrate's perspective. *Chirality*, **2005**, 17 Suppl, S30-9	2.1	32
8	Quantum Reaction Dynamics for Multiple Electronic States. *Advances in Chemical Physics*, **2003**, 283-322		20
7	Towards a general model for protein-substrate stereoselectivity. *Protein Science*, **2002**, 11, 1330-9	6.3	26
6	An optimal adiabatic-to-diabatic transformation of the 1 2A? and 2 2A? states of H3. *Journal of Chemical Physics*, **2002**, 116, 1035-1062	3.9	81
5	Accurate first-derivative nonadiabatic couplings for the H3 system. *Journal of Chemical Physics*, **2001**, 115, 4640-4659	3.9	59
4	A quantum and semiclassical study of dynamical resonances in the C+NO-£N+O reaction. *Journal of Chemical Physics*, **2001**, 114, 7461-7470	3.9	10
3	Reduced potential energy curves for diatomic molecules and their respective cations. *Chemical Physics Letters*, **1999**, 312, 341-345	2.5	1
2	Computation of Vapor Pressure. *Journal of Chemical Education*, **1995**, 72, 1083	2.4	
1	7-Transmembrane Helical (7TMH) Proteins: Pseudo-Symmetry and Conformational Plasticity		1