Harel Weinstein

List of Publications by Year in Descending Order

301 papers	17,175 citations	67 h-index	121 g-index
374 ext. papers	18,720 ext. citations	6 avg, IF	6.68 L-index

#	Paper	IF	Citations
301	Phosphatidylinositol Phosphates Modulate Interactions between the StarD4 Sterol Trafficking Protein and Lipid Membranes. *Journal of Biological Chemistry*, **2022**, 102058	5.4	1
300	Ca -dependent mechanism of membrane insertion and destabilization by the SARS-CoV-2 fusion peptide **2021**,		1
299	Localization atomic force microscopy. *Nature*, **2021**, 594, 385-390	50.4	20
298	A Graphic Encoding Method for Quantitative Classification of Protein Structure and Representation of Conformational Changes. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **2021**, 18, 1336-1349	3	3
297	A lightweight method for evaluating in situ workflow efficiency. *Journal of Computational Science*, **2021**, 48, 101259	3.4	1
296	Elucidating the Mechanism of Membrane Destabilization by the Preferred Modes of Insertion of the Sars-Cov2 Fusion Peptide. *Biophysical Journal*, **2021**, 120, 110a	2.9	78
295	A Machine Learning Algorithm for the Detection of Function-Related Rare Events in MD Trajectories of Biomolecular Systems. *Biophysical Journal*, **2021**, 120, 301a	2.9	3
294	Ca-dependent mechanism of membrane insertion and destabilization by the SARS-CoV-2 fusion peptide. *Biophysical Journal*, **2021**, 120, 1105-1119	2.9	21
293	Use of paramagnetic F NMR to monitor domain movement in a glutamate transporter homolog. *Nature Chemical Biology*, **2020**, 16, 1006-1012	11.7	14
292	X-ray structure of LeuT in an inward-facing occluded conformation reveals mechanism of substrate release. *Nature Communications*, **2020**, 11, 1005	17.4	15
291	Substrate-selective protein ectodomain shedding by ADAM17 and iRhom2 depends on their juxtamembrane and transmembrane domains. *FASEB Journal*, **2020**, 34, 4956-4969	0.9	11
290	A Novel Metric to Evaluate In Situ Workflows. *Lecture Notes in Computer Science*, **2020**, 538-553	0.9	0
289	The Role of Direct Effects of Drugs of Abuse Binding to the hDAT Molecule in their Diverse Behavioral Phenotypes. *FASEB Journal*, **2020**, 34, 1-1	0.9	
288	Structural Basis of Lipid Scrambling and Ion Conduction by TMEM16 Scramblases. *FASEB Journal*, **2020**, 34, 1-1	0.9	
287	Membrane lipids are both the substrates and a mechanistically responsive environment of TMEM16 scramblase proteins. *Journal of Computational Chemistry*, **2020**, 41, 538-551	3.5	6
286	GPCRmd uncovers the dynamics of the 3D-GPCRome. *Nature Methods*, **2020**, 17, 777-787	21.6	34
285	A New Computational Method for Membrane Compressibility: Bilayer Mechanical Thickness Revisited. *Biophysical Journal*, **2019**, 116, 487-502	2.9	34

284	A Machine Learning Approach for the Discovery of Ligand-Specific Functional Mechanisms of GPCRs. *Molecules*, **2019**, 24,	4.8	19
283	Gramicidin Increases Lipid Flip-Flop in Symmetric and Asymmetric Lipid Vesicles. *Biophysical Journal* , **2019**, 116, 860-873	2.9	31
282	Channelrhodopsin-2 Function is Modulated by Residual Hydrophobic Mismatch with the Surrounding Lipid Environment. *Applied Sciences (Switzerland)*, **2019**, 9, 2674	2.6	1
281	Dynamic modulation of the lipid translocation groove generates a conductive ion channel in Ca-bound nhTMEM16. *Nature Communications*, **2019**, 10, 4972	17.4	10
280	The allosteric mechanism of substrate-specific transport in SLC6 is mediated by a volumetric sensor. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 15947-15956	11.5	16
279	A partially-open inward-facing intermediate conformation of LeuT is associated with Na release and substrate transport. *Nature Communications*, **2018**, 9, 230	17.4	28
278	Mechanisms of Lipid Scrambling by the G Protein-Coupled Receptor Opsin. *Structure*, **2018**, 26, 356-367.e3	5.2	35
277	How structural elements evolving from bacterial to human SLC6 transporters enabled new functional properties. *BMC Biology*, **2018**, 16, 31	7.3	25
276	Gating mechanism of the extracellular entry to the lipid pathway in a TMEM16 scramblase. *Nature Communications*, **2018**, 9, 3251	17.4	51
275	The LeuT-fold neurotransmitter:sodium symporter MhsT has two substrate sites. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E7924-E7931	11.5	14
274	Thermodynamic Coupling Function Analysis of Allosteric Mechanisms in the Human Dopamine Transporter. *Biophysical Journal*, **2018**, 114, 10-14	2.9	11
273	Graphic Encoding of Macromolecules for Efficient High-Throughput Analysis **2018**,		3
272	Accurate In Silico Modeling of Asymmetric Bilayers Based on Biophysical Principles. *Biophysical Journal*, **2018**, 115, 1638-1643	2.9	26
271	An Amphipathic Helix Directs Cellular Membrane Curvature Sensing and Function of the BAR Domain Protein PICK1. *Cell Reports*, **2018**, 23, 2056-2069	10.6	21
270	Structural modeling defines transmembrane residues in ADAM17 that are crucial for Rhbdf2-ADAM17-dependent proteolysis. *Journal of Cell Science*, **2017**, 130, 868-878	5.3	25
269	A Markov State-based Quantitative Kinetic Model of Sodium Release from the Dopamine Transporter. *Scientific Reports*, **2017**, 7, 40076	4.9	46
268	Single-molecule analysis of ligand efficacy in β2AR-G-protein activation. *Nature*, **2017**, 547, 68-73	50.4	164
267	The role of transmembrane segment 5 (TM5) in Na2 release and the conformational transition of neurotransmitter:sodium symporters toward the inward-open state. *Journal of Biological Chemistry*, **2017**, 292, 7372-7384	5.4	17

266	Combined in vitro and in silico approaches to the assessment of stimulant properties of novel psychoactive substances - The case of the benzofuran 5-MAPB. *Progress in Neuro-Psychopharmacology and Biological Psychiatry*, **2017**, 75, 1-9	5.5	16
265	Evolutionary Divergence of the C-terminal Domain of Complexin Accounts for Functional Disparities between Vertebrate and Invertebrate Complexins. *Frontiers in Molecular Neuroscience*, **2017**, 10, 146	6.1	13
264	Conformational Dynamics on the Extracellular Side of LeuT Controlled by Na+ and K+ Ions and the Protonation State of Glu290. *Journal of Biological Chemistry*, **2016**, 291, 19786-99	5.4	16
263	Augmenting drug-carrier compatibility improves tumour nanotherapy efficacy. *Nature Communications*, **2016**, 7, 11221	17.4	96
262	The Allostery Landscape: Quantifying Thermodynamic Couplings in Biomolecular Systems. *Journal of Chemical Theory and Computation*, **2016**, 12, 5758-5767	6.4	20
261	Role of Annular Lipids in the Functional Properties of Leucine Transporter LeuT Proteomicelles. *Biochemistry*, **2016**, 55, 850-9	3.2	10
260	Computational approaches to detect allosteric pathways in transmembrane molecular machines. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1652-62	3.8	38
259	Allosteric Mechanisms of Molecular Machines at the Membrane: Transport by Sodium-Coupled Symporters. *Chemical Reviews*, **2016**, 116, 6552-87	68.1	59
258	A GIPC1-Palmitate Switch Modulates Dopamine Drd3 Receptor Trafficking and Signaling. *Molecular and Cellular Biology*, **2016**, 36, 1019-31	4.8	8
257	A mechanistic role of Helix 8 in GPCRs: Computational modeling of the dopamine D2 receptor interaction with the GIPC1-PDZ-domain. *Biochimica Et Biophysica Acta - Biomembranes*, **2015**, 1848, 976-83	3.8	31
256	AIM for Allostery: Using the Ising Model to Understand Information Processing and Transmission in Allosteric Biomolecular Systems. *Entropy*, **2015**, 17, 2895-2918	2.8	13
255	Structure of Dimeric and Tetrameric Complexes of the BAR Domain Protein PICK1 Determined by Small-Angle X-Ray Scattering. *Structure*, **2015**, 23, 1258-1270	5.2	24
254	Functional mechanisms of neurotransmitter transporters regulated by lipid-protein interactions of their terminal loops. *Biochimica Et Biophysica Acta - Biomembranes*, **2015**, 1848, 1765-74	3.8	22
253	Substrate-induced unlocking of the inner gate determines the catalytic efficiency of a neurotransmitter:sodium symporter. *Journal of Biological Chemistry*, **2015**, 290, 26725-38	5.4	28
252	Spontaneous inward opening of the dopamine transporter is triggered by PIP2-regulated dynamics of the N-terminus. *ACS Chemical Neuroscience*, **2015**, 6, 1825-37	5.7	75
251	Mechanism of the Association between Na+ Binding and Conformations at the Intracellular Gate in Neurotransmitter:Sodium Symporters. *Journal of Biological Chemistry*, **2015**, 290, 13992-4003	5.4	41
250	Computational Modeling of the N-Terminus of the Human Dopamine Transporter (hDAT). *Biophysical Journal*, **2015**, 108, 252a	2.9	2
249	Computational modeling of the N-terminus of the human dopamine transporter and its interaction with PIP2 -containing membranes. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 952-69	4.2	39

248	Transport domain unlocking sets the uptake rate of an aspartate transporter. *Nature*, **2015**, 518, 68-73	50.4	120
247	The second sodium site in the dopamine transporter controls cation permeation and is regulated by chloride. *Journal of Biological Chemistry*, **2014**, 289, 25764-73	5.4	30
246	A functional selectivity mechanism at the serotonin-2A GPCR involves ligand-dependent conformations of intracellular loop 2. *Journal of the American Chemical Society*, **2014**, 136, 16044-54	16.4	55
245	Protein and lipid interactions driving molecular mechanisms of in meso crystallization. *Journal of the American Chemical Society*, **2014**, 136, 3271-84	16.4	15
244	Not just an oil slick: how the energetics of protein-membrane interactions impacts the function and organization of transmembrane proteins. *Biophysical Journal*, **2014**, 106, 2305-16	2.9	46
243	PIP2 regulates psychostimulant behaviors through its interaction with a membrane protein. *Nature Chemical Biology*, **2014**, 10, 582-589	11.7	83
242	Conformational dynamics of ligand-dependent alternating access in LeuT. *Nature Structural and Molecular Biology*, **2014**, 21, 472-9	17.6	102
241	NbIT--a new information theory-based analysis of allosteric mechanisms reveals residues that underlie function in the leucine transporter LeuT. *PLoS Computational Biology*, **2014**, 10, e1003603	5	68
240	ESCRT-II/Vps25 constrains digit number by endosome-mediated selective modulation of FGF-SHH signaling. *Cell Reports*, **2014**, 9, 674-87	10.6	8
239	Conformational changes in dopamine transporter intracellular regions upon cocaine binding and dopamine translocation. *Neurochemistry International*, **2014**, 73, 4-15	4.4	10
238	Missense dopamine transporter mutations associate with adult parkinsonism and ADHD. *Journal of Clinical Investigation*, **2014**, 124, 3107-20	15.9	80
237	How the dynamic properties and functional mechanisms of GPCRs are modulated by their coupling to the membrane environment. *Advances in Experimental Medicine and Biology*, **2014**, 796, 55-74	3.6	21
236	Membrane driven spatial organization of GPCRs. *Scientific Reports*, **2013**, 3, 2909	4.9	86
235	The membrane protein LeuT in micellar systems: aggregation dynamics and detergent binding to the S2 site. *Journal of the American Chemical Society*, **2013**, 135, 14266-75	16.4	29
234	The cost of living in the membrane: a case study of hydrophobic mismatch for the multi-segment protein LeuT. *Chemistry and Physics of Lipids*, **2013**, 169, 27-38	3.7	38
233	Chloride binding site of neurotransmitter sodium symporters. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 8489-94	11.5	65
232	Turkey must end violent response to protests. *Science*, **2013**, 341, 236	33.3	2
231	Experimental conditions can obscure the second high-affinity site in LeuT. *Nature Structural and Molecular Biology*, **2012**, 19, 207-11	17.6	82

230	Interaction with the Membrane Uncovers Essential Differences Between Highly Homologous GPCRs. *Biophysical Journal*, **2012**, 102, 514a	2.9	2
229	Why GPCRs behave differently in cubic and lamellar lipidic mesophases. *Journal of the American Chemical Society*, **2012**, 134, 15858-68	16.4	44
228	Phosphatidylinositol 4,5-biphosphate (PIP(2)) lipids regulate the phosphorylation of syntaxin N-terminus by modulating both its position and local structure. *Biochemistry*, **2012**, 51, 7685-98	3.2	21
227	Structural intermediates in a model of the substrate translocation path of the bacterial glutamate transporter homologue GltPh. *Journal of Physical Chemistry B*, **2012**, 116, 5372-83	3.4	40
226	Ion-controlled conformational dynamics in the outward-open transition from an occluded state of LeuT. *Biophysical Journal*, **2012**, 103, 878-88	2.9	77
225	9.12 Interactions of the Cell Membrane with Integral Proteins **2012**, 229-242		2
224	Structural Intermediates in a Model of the Substrate Translocation Path in the Bacterial Glutamate Transporter Homologue GltPh. *Biophysical Journal*, **2012**, 102, 519a	2.9	2
223	In support of the BMRB. *Nature Structural and Molecular Biology*, **2012**, 19, 854-60	17.6	5
222	9.1 Theoretical Biophysics: A Cornerstone of Understanding in Modern Biology and Biomedicine **2012**, 1		
221	Ligand-dependent conformations and dynamics of the serotonin 5-HT(2A) receptor determine its activation and membrane-driven oligomerization properties. *PLoS Computational Biology*, **2012**, 8, e1002473	5	84
220	Steric hindrance mutagenesis in the conserved extracellular vestibule impedes allosteric binding of antidepressants to the serotonin transporter. *Journal of Biological Chemistry*, **2012**, 287, 39316-26	5.4	74
219	Pharmacologically Distinct Ligands Induce Different States of 5-HT2AR and Trigger Different Membrane Remodeling: Implications For GPCR Oligomerization. *Biophysical Journal*, **2011**, 100, 254a	2.9	4
218	Quantitative modeling of membrane deformations by multihelical membrane proteins: application to G-protein coupled receptors. *Biophysical Journal*, **2011**, 101, 2092-101	2.9	76
217	The correlation between multidomain enzymes and multiple activation mechanisms--the case of phospholipase C□and its membrane interactions. *Biochimica Et Biophysica Acta - Biomembranes*, **2011**, 1808, 2940-7	3.8	7
216	PDZ binding to the BAR domain of PICK1 is elucidated by coarse-grained molecular dynamics. *Journal of Molecular Biology*, **2011**, 405, 298-314	6.5	34
215	The binding sites for benztropines and dopamine in the dopamine transporter overlap. *Neuropharmacology*, **2011**, 60, 182-90	5.5	49
214	Substrate-modulated gating dynamics in a Na+-coupled neurotransmitter transporter homologue. *Nature*, **2011**, 474, 109-13	50.4	244
213	A dynamic model of membrane-bound phospholipase C□ activation by G□subunits. *Molecular Pharmacology*, **2011**, 80, 434-45	4.3	18

212	The substrate-driven transition to an inward-facing conformation in the functional mechanism of the dopamine transporter. *PLoS ONE*, **2011**, 6, e16350	3.7	99
211	Ion/substrate-dependent conformational dynamics of a bacterial homolog of neurotransmitter:sodium symporters. *Nature Structural and Molecular Biology*, **2010**, 17, 822-9	17.6	157
210	Single-molecule dynamics of gating in a neurotransmitter transporter homologue. *Nature*, **2010**, 465, 188-93	50.4	213
209	Substrate-dependent proton antiport in neurotransmitter:sodium symporters. *Nature Chemical Biology*, **2010**, 6, 109-16	11.7	48
208	Identification of a small-molecule inhibitor of the PICK1 PDZ domain that inhibits hippocampal LTP and LTD. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 413-8	11.5	86
207	Conformational rearrangements to the intracellular open states of the LeuT and ApcT transporters are modulated by common mechanisms. *Biophysical Journal*, **2010**, 99, L103-5	2.9	41
206	Cholesterol modulates the membrane effects and spatial organization of membrane-penetrating ligands for G-protein coupled receptors. *Journal of Physical Chemistry B*, **2010**, 114, 12046-57	3.4	30
205	Structure-activity relationships of a small-molecule inhibitor of the PDZ domain of PICK1. *Organic and Biomolecular Chemistry*, **2010**, 8, 4281-8	3.9	28
204	Probing the structural determinants for the function of intracellular loop 2 in structurally cognate G-protein-coupled receptors. *Biochemistry*, **2010**, 49, 10691-701	3.2	16
203	TRAC: A Platform for Structure-Function Studies of NSS-Proteins Integrates Information from Bioinformatics and Biomedical Literature **2010**,		1
202	Structural Basis of Dopamine Receptor Activation **2010**, 47-73		3
201	Ligand selectivity of D2 dopamine receptors is modulated by changes in local dynamics produced by sodium binding. *Journal of Pharmacology and Experimental Therapeutics*, **2009**, 328, 40-54	4.7	29
200	Binding of an octylglucoside detergent molecule in the second substrate (S2) site of LeuT establishes an inhibitor-bound conformation. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 5563-8	11.5	160
199	A juxtamembrane mutation in the N terminus of the dopamine transporter induces preference for an inward-facing conformation. *Molecular Pharmacology*, **2009**, 75, 514-24	4.3	56
198	Structural and dynamic effects of cholesterol at preferred sites of interaction with rhodopsin identified from microsecond length molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2009**, 76, 403-17	4.2	100
197	Models for molecular mechanisms in drug–receptor interactions. Serotonin and 5-hydroxyindole complexes with imidazolium cation. *International Journal of Quantum Chemistry*, **2009**, 12, 253-268	2.1	
196	Theoretical models for molecular mechanisms in biological systems: Tryptamine congeners acting on an LSD–serotonin receptor. *International Journal of Quantum Chemistry*, **2009**, 14, 449-461	2.1	
195	The solvent effect in enzyme–substrate interactions: Models of carboxypeptidase. *International Journal of Quantum Chemistry*, **2009**, 22, 355-365	2.1	

194	Theoretical studies on the activation mechanism of the histamine H2-receptor: The guanidine substitution and its role in the partial agonism of N(alpha)-guanylhistamine. *International Journal of Quantum Chemistry*, **2009**, 24, 293-300	2.1	1
193	Molecular determinants for recognition of phencyclidine derivatives at muscarinic cholinergic receptors. *International Journal of Quantum Chemistry*, **2009**, 24, 309-320	2.1	
192	Theoretical studies of the activation mechanism of histamine H2-receptors: Dimaprit and the receptor model. *International Journal of Quantum Chemistry*, **2009**, 36, 281-290	2.1	
191	Some new quantum chemical procedures for the analysis of drug□eceptor interactions. *International Journal of Quantum Chemistry*, **2009**, 9, 59-69	2.1	
190	Reactivity characteristics of large molecules and their biological activity: Indolealkylamines on the LSD/serotonin receptor. *International Journal of Quantum Chemistry*, **2009**, 10, 135-150	2.1	
189	Allosteric communication between protomers of dopamine class A GPCR dimers modulates activation. *Nature Chemical Biology*, **2009**, 5, 688-95	11.7	294
188	Towards a quantitative representation of the cell signaling mechanisms of hallucinogens: measurement and mathematical modeling of 5-HT1A and 5-HT2A receptor-mediated ERK1/2 activation. *Neuropharmacology*, **2009**, 56 Suppl 1, 213-25	5.5	19
187	Modeling membrane deformations and lipid demixing upon protein-membrane interaction: the BAR dimer adsorption. *Biophysical Journal*, **2009**, 97, 1626-35	2.9	55
186	Probing the Dynamic Structure and Function of Intracellular Loop 2 in Structurally Cognate GPCRs. *Biophysical Journal*, **2009**, 96, 429a-430a	2.9	1
185	The binding sites for cocaine and dopamine in the dopamine transporter overlap. *Nature Neuroscience*, **2008**, 11, 780-9	25.5	260
184	Mutations affecting the oligomerization interface of G-protein-coupled receptors revealed by a novel de novo protein design framework. *Biophysical Journal*, **2008**, 94, 2470-81	2.9	22
183	Protein diffusion on charged membranes: a dynamic mean-field model describes time evolution and lipid reorganization. *Biophysical Journal*, **2008**, 94, 2580-97	2.9	49
182	The mechanism of a neurotransmitter:sodium symporter--inward release of Na+ and substrate is triggered by substrate in a second binding site. *Molecular Cell*, **2008**, 30, 667-77	17.6	308
181	Active state-like conformational elements in the beta2-AR and a photoactivated intermediate of rhodopsin identified by dynamic properties of GPCRs. *Biochemistry*, **2008**, 47, 7317-21	3.2	18
180	Effects of tobacco smoke on gene expression and cellular pathways in a cellular model of oral leukoplakia. *Cancer Prevention Research*, **2008**, 1, 100-11	3.2	47
179	An intracellular interaction network regulates conformational transitions in the dopamine transporter. *Journal of Biological Chemistry*, **2008**, 283, 17691-701	5.4	108
178	Identification of GATC- and CCGG-recognizing Type II REases and their putative specificity-determining positions using Scan2S--a novel motif scan algorithm with optional secondary structure constraints. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 631-40	4.2	2
177	Membrane localization is critical for activation of the PICK1 BAR domain. *Traffic*, **2008**, 9, 1327-43	5.7	41

176	Hallucinogen Actions on 5-HT Receptors Reveal Distinct Mechanisms of Activation and Signaling by G Protein-Coupled Receptors **2008**, 265-286		
175	Sodium-induced allosteric changes in D2 dopamine receptor local dynamics modulate ligand selectivity. *FASEB Journal*, **2008**, 22, 727.4	0.9	
174	Topology of Type II REases revisited; structural classes and the common conserved core. *Nucleic Acids Research*, **2007**, 35, 2227-37	20.1	32
173	Functional selectivity and classical concepts of quantitative pharmacology. *Journal of Pharmacology and Experimental Therapeutics*, **2007**, 320, 1-13	4.7	870
172	Toward realistic modeling of dynamic processes in cell signaling: quantification of macromolecular crowding effects. *Journal of Chemical Physics*, **2007**, 127, 155105	3.9	55
171	State-dependent conformations of the translocation pathway in the tyrosine transporter Tyt1, a novel neurotransmitter:sodium symporter from Fusobacterium nucleatum. *Journal of Biological Chemistry*, **2006**, 281, 26444-54	5.4	77
170	A comprehensive structure-based alignment of prokaryotic and eukaryotic neurotransmitter/Na+ symporters (NSS) aids in the use of the LeuT structure to probe NSS structure and function. *Molecular Pharmacology*, **2006**, 70, 1630-42	4.3	232
169	Trefoil factor family-1 mutations enhance gastric cancer cell invasion through distinct signaling pathways. *Gastroenterology*, **2006**, 130, 1696-706	13.3	33
168	Thermodynamic basis for promiscuity and selectivity in protein-protein interactions: PDZ domains, a case study. *Journal of the American Chemical Society*, **2006**, 128, 12766-77	16.4	96
167	Ab initio computational modeling of loops in G-protein-coupled receptors: lessons from the crystal structure of rhodopsin. *Proteins: Structure, Function and Bioinformatics*, **2006**, 64, 673-90	4.2	35
166	Dynamic models of G-protein coupled receptor dimers: indications of asymmetry in the rhodopsin dimer from molecular dynamics simulations in a POPC bilayer. *Journal of Computer-Aided Molecular Design*, **2006**, 20, 405-16	4.2	59
165	Modeling activated states of GPCRs: the rhodopsin template. *Journal of Computer-Aided Molecular Design*, **2006**, 20, 437-48	4.2	62
164	Hallucinogen actions on 5-HT receptors reveal distinct mechanisms of activation and signaling by G protein-coupled receptors. *AAPS Journal*, **2006**, 7, E871-84	3.7	27
163	Transmembrane five effects on functional selectivity at the dopamine D2L receptor. *FASEB Journal*, **2006**, 20, A246	0.9	
162	A flexible docking procedure for the exploration of peptide binding selectivity to known structures and homology models of PDZ domains. *Journal of the American Chemical Society*, **2005**, 127, 14072-9	16.4	63
161	Oligomerization Domains of G Protein-Coupled Receptors **2005**, 243-265		4
160	A pincer-like configuration of TM2 in the human dopamine transporter is responsible for indirect effects on cocaine binding. *Neuropharmacology*, **2005**, 49, 780-90	5.5	36
159	PDZBase: a protein-protein interaction database for PDZ-domains. *Bioinformatics*, **2005**, 21, 827-8	7.2	160

158	The study of G-protein coupled receptor oligomerization with computational modeling and bioinformatics. *FEBS Journal*, **2005**, 272, 2926-38	5.7	87
157	Epilogue: New Levels of Complexity in the Functional Roles of Modular Protein Interaction Domains: Switches and Sockets in the Circuit Diagrams of Cellular Systems Biology **2005**, 487-491		
156	Crosstalk in G protein-coupled receptors: changes at the transmembrane homodimer interface determine activation. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 17495-500	11.5	252
155	Modeling membrane proteins based on low-resolution electron microscopy maps: a template for the TM domains of the oxalate transporter OxlT. *Protein Engineering, Design and Selection*, **2005**, 18, 119-25	1.9	14
154	Molecular determinants for the complex binding specificity of the PDZ domain in PICK1. *Journal of Biological Chemistry*, **2005**, 280, 20539-48	5.4	61
153	Crooked tail (Cd) model of human folate-responsive neural tube defects is mutated in Wnt coreceptor lipoprotein receptor-related protein 6. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 12843-8	11.5	81
152	The structure and dynamics of GPCR oligomers: a new focus in models of cell-signaling mechanisms and drug design. *Current Opinion in Drug Discovery & Development*, **2005**, 8, 577-84		15
151	Mechanistic insights from a refined three-dimensional model of integrin alphaIIbbeta3. *Journal of Biological Chemistry*, **2004**, 279, 24624-30	5.4	9
150	Certain 1,4-disubstituted aromatic piperidines and piperazines with extreme selectivity for the dopamine D4 receptor interact with a common receptor microdomain. *Molecular Pharmacology*, **2004**, 66, 1491-9	4.3	36
149	A knowledge-based scale for the analysis and prediction of buried and exposed faces of transmembrane domain proteins. *Bioinformatics*, **2004**, 20, 1822-35	7.2	66
148	Quantitative information management for the biochemical computation of cellular networks. *Science Signaling*, **2004**, 2004, pl11	8.8	26
147	Surface Tension Parameterization in Molecular Dynamics Simulations of a Phospholipid-bilayer Membrane: Calibration and Effects. *Journal of Physical Chemistry B*, **2004**, 108, 11802-11811	3.4	20
146	Molecular dynamics simulations of transducin: interdomain and front to back communication in activation and nucleotide exchange. *Journal of Molecular Biology*, **2004**, 338, 469-81	6.5	40
145	A Structural Context for Studying Neurotransmitter Transporter Function **2004**, 213-234		1
144	Functional Mechanisms of G Protein-Coupled Receptors in a Structural Context **2004**, 235-266		3
143	Molecular basis of partial agonism: orientation of indoleamine ligands in the binding pocket of the human serotonin 5-HT2A receptor determines relative efficacy. *Molecular Pharmacology*, **2003**, 63, 36-43	4.3	62
142	Probing conformational changes in neurotransmitter transporters: a structural context. *European Journal of Pharmacology*, **2003**, 479, 3-12	5.3	36
141	Molecular dynamics simulations of peptides and proteins with a continuum electrostatic model based on screened Coulomb potentials. *Proteins: Structure, Function and Bioinformatics*, **2003**, 51, 109-25	4.2	59

140	A second site rescue mutation partially restores functional expression to the serotonin transporter mutant V382P. *Biochemistry*, **2003**, 42, 6784-93	3.2	7
139	Energetic and structural considerations for the mechanism of protein sliding along DNA in the nonspecific BamHI-DNA complex. *Biophysical Journal*, **2003**, 84, 3317-25	2.9	26
138	Building protein diagrams on the web with the residue-based diagram editor RbDe. *Nucleic Acids Research*, **2003**, 31, 3856-8	20.1	22
137	Batch mode generation of residue-based diagrams of proteins. *Bioinformatics*, **2003**, 19, 1854-5	7.2	8
136	Structural models for dimerization of G-protein coupled receptors: the opioid receptor homodimers. *Biopolymers*, **2002**, 66, 317-25	2.2	76
135	Structural motifs as functional microdomains in G-protein-coupled receptors: Energetic considerations in the mechanism of activation of the serotonin 5-HT2A receptor by disruption of the ionic lock of the arginine cage*. *International Journal of Quantum Chemistry*, **2002**, 88, 65-75	2.1	42
134	Key issues in the computational simulation of GPCR function: representation of loop domains. *Journal of Computer-Aided Molecular Design*, **2002**, 16, 841-53	4.2	48
133	Conserved helix 7 tyrosine acts as a multistate conformational switch in the 5HT2C receptor. Identification of a novel "locked-on" phenotype and double revertant mutations. *Journal of Biological Chemistry*, **2002**, 277, 36577-84	5.4	99
132	Three-dimensional representations of G protein-coupled receptor structures and mechanisms. *Methods in Enzymology*, **2002**, 343, 329-71	1.7	143
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