Emad Tajkhorshid

List of Publications by Year in Descending Order

275 papers	27,001 citations	67 h-index	161 g-index
335 ext. papers	31,490 ext. citations	7.7 avg, IF	6.96 L-index

#	Paper	IF	Citations
275	Identification of Structural transitions in bacterial fatty acid binding proteins that permit ligand entry and exit at membranes.. *Journal of Biological Chemistry*, **2022**, 101676	5.4	4
274	Anthracycline derivatives inhibit cardiac CYP2J2.. *Journal of Inorganic Biochemistry*, **2022**, 229, 111722	4.2	0
273	Extended-ensemble docking to probe dynamic variation of ligand binding sites during large-scale structural changes of proteins.. *Chemical Science*, **2022**, 13, 4150-4169	9.4	3
272	Role of internal loop dynamics in antibiotic permeability of outer membrane porins.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119,	11.5	1
271	Rationalizing the generation of broad spectrum antibiotics with the addition of a positive charge.. *Chemical Science*, **2021**, 12, 15028-15044	9.4	3
270	PIP-dependent coupling of voltage sensor and pore domains in K7.2 channel. *Communications Biology*, **2021**, 4, 1189	6.7	0
269	Binding mode of SARS-CoV-2 fusion peptide to human cellular membrane. *Biophysical Journal*, **2021** , 120, 2914-2926	2.9	10
268	Structural insights into photosystem II assembly. *Nature Plants*, **2021**, 7, 524-538	11.5	31
267	Defining the Energetic Basis for a Conformational Switch Mediating Ligand-Independent Activation of Mutant Estrogen Receptors in Breast Cancer. *Molecular Cancer Research*, **2021**, 19, 1559-1570	6.6	1
266	Mechanical properties of ester- and ether-DPhPC bilayers: A molecular dynamics study. *Journal of the Mechanical Behavior of Biomedical Materials*, **2021**, 117, 104386	4.1	0
265	Structural basis of complex formation between mitochondrial anion channel VDAC1 and Hexokinase-II. *Communications Biology*, **2021**, 4, 667	6.7	4
264	Conformational changes in the nucleotide-binding domains of P-glycoprotein induced by ATP hydrolysis. *FEBS Letters*, **2021**, 595, 735-749	3.8	4
263	Calmodulin complexes with brain and muscle creatine kinase peptides. *Current Research in Structural Biology*, **2021**, 3, 121-132	2.8	1
262	GOLEM: Automated and Robust Cryo-EM-Guided Ligand Docking with Explicit Water Molecules. *Biophysical Journal*, **2021**, 120, 290a	2.9	2
261	Glutamate transporters have a chloride channel with two hydrophobic gates. *Nature*, **2021**, 591, 327-331	50.4	13
260	Anti-inflammatory dopamine- and serotonin-based endocannabinoid epoxides reciprocally regulate cannabinoid receptors and the TRPV1 channel. *Nature Communications*, **2021**, 12, 926	17.4	3
259	Carbon dioxide transport across membranes. *Interface Focus*, **2021**, 11, 20200090	3.9	5

258	Amphiphilic Distyrylbenzene Derivatives as Potential Therapeutic and Imaging Agents for Soluble and Insoluble Amyloid Aggregates in Alzheimer's Disease. *Journal of the American Chemical Society*, **2021**, 143, 10462-10476	16.4	6
257	Molecular mechanism of capsid disassembly in hepatitis B virus. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	3
256	Cryo-EM structures of cytochrome reveal bound phospholipids and ubiquinone-8 in a dynamic substrate binding site. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	6
255	Cation- Interactions and their Functional Roles in Membrane Proteins. *Journal of Molecular Biology* , **2021**, 433, 167035	6.5	6
254	Differential Interactions of Selected Phytocannabinoids with Human CYP2D6 Polymorphisms. *Biochemistry*, **2021**, 60, 2749-2760	3.2	1
253	Molecular mechanism of prestin electromotive signal amplification. *Cell*, **2021**, 184, 4669-4679.e13	56.2	10
252	CryoFold: Determining protein structures and data-guided ensembles from cryo-EM density maps. *Matter*, **2021**,	12.7	2
251	Active participation of membrane lipids in inhibition of multidrug transporter P-glycoprotein. *Chemical Science*, **2021**, 12, 6293-6306	9.4	6
250	Assembly and Analysis of Cell-Scale Membrane Envelopes.. *Journal of Chemical Information and Modeling*, **2021**,	6.1	2
249	An Allosteric Binding Site on Sortilin Regulates the Trafficking of VLDL, PCSK9, and LDLR in Hepatocytes. *Biochemistry*, **2020**, 59, 4321-4335	3.2	3
248	Twisting and tilting of a mechanosensitive molecular probe detects order in membranes. *Chemical Science*, **2020**, 11, 5637-5649	9.4	9
247	A(1-42) tetramer and octamer structures reveal edge conductivity pores as a mechanism for membrane damage. *Nature Communications*, **2020**, 11, 3014	17.4	77
246	Identifying mutation hotspots reveals pathogenetic mechanisms of KCNQ2 epileptic encephalopathy. *Scientific Reports*, **2020**, 10, 4756	4.9	18
245	Aquaporin-7: A Dynamic Aquaglyceroporin With Greater Water and Glycerol Permeability Than Its Bacterial Homolog GlpF. *Frontiers in Physiology*, **2020**, 11, 728	4.6	13
244	Aberrant Expression of a Non-muscle RBFOX2 Isoform Triggers Cardiac Conduction Defects in Myotonic Dystrophy. *Developmental Cell*, **2020**, 52, 748-763.e6	10.2	13
243	Menthol Binding to the Human 42 Nicotinic Acetylcholine Receptor Facilitated by Its Strong Partitioning in the Membrane. *Journal of Physical Chemistry B*, **2020**, 124, 1866-1880	3.4	5
242	Molecular Insights into the Loading and Dynamics of Doxorubicin on PEGylated Graphene Oxide Nanocarriers. *ACS Applied Bio Materials*, **2020**, 3, 1354-1363	4.1	26
241	Microscopic Characterization of GRP1 PH Domain Interaction with Anionic Membranes. *Journal of Computational Chemistry*, **2020**, 41, 489-499	3.5	16

240	Knockout of VDAC1 in H9c2 Cells Promotes Oxidative Stress-Induced Cell Apoptosis through Decreased Mitochondrial Hexokinase II Binding and Enhanced Glycolytic Stress. *Cellular Physiology and Biochemistry*, **2020**, 54, 853-874	3.9	2
239	A CLC-ec1 mutant reveals global conformational change and suggests a unifying mechanism for the CLC Cl/H transport cycle. *ELife*, **2020**, 9,	8.9	17
238	The structures of secretory and dimeric immunoglobulin A. *ELife*, **2020**, 9,	8.9	9
237	Structural basis for the reaction cycle of DASS dicarboxylate transporters. *ELife*, **2020**, 9,	8.9	18
236	Confronting pitfalls of AI-augmented molecular dynamics using statistical physics. *Journal of Chemical Physics*, **2020**, 153, 234118	3.9	4
235	Probing cholesterol binding and translocation in P-glycoprotein. *Biochimica Et Biophysica Acta - Biomembranes*, **2020**, 1862, 183090	3.8	6
234	An Activity-Based Sensing Approach for the Detection of Cyclooxygenase-2 in Live Cells. *Angewandte Chemie*, **2020**, 132, 3333-3340	3.6	13
233	Cryo-EM structures of a lipid-sensitive pentameric ligand-gated ion channel embedded in a phosphatidylcholine-only bilayer. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 1788-1798	11.5	19
232	An Activity-Based Sensing Approach for the Detection of Cyclooxygenase-2 in Live Cells. *Angewandte Chemie - International Edition*, **2020**, 59, 3307-3314	16.4	31
231	Computational Dissection of Membrane Transport at a Microscopic Level. *Trends in Biochemical Sciences*, **2020**, 45, 202-216	10.3	7
230	Structural and functional diversity calls for a new classification of ABC transporters. *FEBS Letters*, **2020**, 594, 3767-3775	3.8	66
229	Membrane surface recognition by the ASAP1 PH domain and consequences for interactions with the small GTPase Arf1. *Science Advances*, **2020**, 6,	14.3	7
228	Hydrogen-deuterium exchange mass spectrometry captures distinct dynamics upon substrate and inhibitor binding to a transporter. *Nature Communications*, **2020**, 11, 6162	17.4	15
227	Scalable molecular dynamics on CPU and GPU architectures with NAMD. *Journal of Chemical Physics* , **2020**, 153, 044130	3.9	483
226	Membrane Interactions of Cy3 and Cy5 Fluorophores and Their Effects on Membrane-Protein Dynamics. *Biophysical Journal*, **2020**, 119, 24-34	2.9	7
225	Parameterization of a drug molecule with a halogen ℎole particle using ffTK: Implementation, testing, and comparison. *Journal of Chemical Physics*, **2020**, 153, 164104	3.9	1
224	Boosting Free-Energy Perturbation Calculations with GPU-Accelerated NAMD. *Journal of Chemical Information and Modeling*, **2020**, 60, 5301-5307	6.1	16
223	Polymer-Peptide Conjugates Convert Amyloid into Protein Nanobundles through Fragmentation and Lateral Association. *ACS Applied Nano Materials*, **2020**, 3, 937-945	5.6	7

222	A network of phosphatidylinositol 4,5-bisphosphate binding sites regulates gating of the Ca-activated Cl channel ANO1 (TMEM16A). *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 19952-19962	11.5	33
221	Multivalent Polymer-Peptide Conjugates-A General Platform for Inhibiting Amyloid Beta Peptide Aggregation. *ACS Macro Letters*, **2019**, 8, 1365-1371	6.6	8
220	Phosphatidic acid induces conformational changes in Sec18 protomers that prevent SNARE priming. *Journal of Biological Chemistry*, **2019**, 294, 3100-3116	5.4	13
219	Structural Insights into the Lipid A Transport Pathway in MsbA. *Structure*, **2019**, 27, 1114-1123.e3	5.2	13
218	Pro-Nifuroxazide Self-Assembly Leads to Triggerable Nanomedicine for Anti-cancer Therapy. *ACS Applied Materials & Interfaces*, **2019**, 11, 18074-18089	9.5	7
217	Serotonin transporter-ibogaine complexes illuminate mechanisms of inhibition and transport. *Nature*, **2019**, 569, 141-145	50.4	89
216	Characterization of Lipid-Protein Interactions and Lipid-Mediated Modulation of Membrane Protein Function through Molecular Simulation. *Chemical Reviews*, **2019**, 119, 6086-6161	68.1	80
215	Allosteric Interactions in Human Cytochrome P450 CYP3A4: The Role of Phenylalanine 213. *Biochemistry*, **2019**, 58, 1411-1422	3.2	12
214	A Chalcogen-Bonding Cascade Switch for Planarizable Push-Pull Probes. *Angewandte Chemie - International Edition*, **2019**, 58, 15752-15756	16.4	30
213	Binding partner- and force-promoted changes in E-catenin conformation probed by native cysteine labeling. *Scientific Reports*, **2019**, 9, 15375	4.9	5
212	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. *Cell*, **2019**, 179, 1098-1111.e23	36.1	23
211	A small-molecule competitive inhibitor of phosphatidic acid binding by the AAA+ protein NSF/Sec18 blocks the SNARE-priming stage of vacuole fusion. *Journal of Biological Chemistry*, **2019**, 294, 17168-17185	5.4	2
210	A Chalcogen-Bonding Cascade Switch for Planarizable PushPull Probes. *Angewandte Chemie*, **2019**, 131, 15899-15903	3.6	12
209	Locking Two Rigid-body Bundles in an Outward-Facing Conformation: The Ion-coupling Mechanism in a LeuT-fold Transporter. *Scientific Reports*, **2019**, 9, 19479	4.9	6
208	Integrating hydrogen-deuterium exchange mass spectrometry with molecular dynamics simulations to probe lipid-modulated conformational changes in membrane proteins. *Nature Protocols*, **2019**, 14, 3183-3204	18.8	22
207	Tuning symmetry breaking charge separation in perylene bichromophores by conformational control. *Chemical Science*, **2019**, 10, 10629-10639	9.4	26
206	Structure of the alternative complex III in a supercomplex with cytochrome oxidase. *Nature*, **2018**, 557, 123-126	50.4	144
205	PyContact: Rapid, Customizable, and Visual Analysis of Noncovalent Interactions in MD Simulations. *Biophysical Journal*, **2018**, 114, 577-583	2.9	39

204	A "cross-stitched" peptide with improved helicity and proteolytic stability. *Organic and Biomolecular Chemistry*, **2018**, 16, 3702-3706	3.9	19
203	Cytochrome aa Oxygen Reductase Utilizes the Tunnel Observed in the Crystal Structures To Deliver O for Catalysis. *Biochemistry*, **2018**, 57, 2150-2161	3.2	3
202	Sensitivity of peripheral membrane proteins to the membrane context: A case study of phosphatidylserine and the TIM proteins. *Biochimica Et Biophysica Acta - Biomembranes*, **2018**, 1860, 2126-2133	3.8	8
201	Reconstitution and substrate specificity for isopentenyl pyrophosphate of the antiviral radical SAM enzyme viperin. *Journal of Biological Chemistry*, **2018**, 293, 14122-14133	5.4	8
200	Microscopic view of lipids and their diverse biological functions. *Current Opinion in Structural Biology*, **2018**, 51, 177-186	8.1	17
199	Probing key elements of teixobactin-lipid II interactions in membranes. *Chemical Science*, **2018**, 9, 6997-7008	9.1	15
198	Electrostatic lock in the transport cycle of the multidrug resistance transporter EmrE. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E7502-E7511	11.5	21
197	Constructing atomic structural models into cryo-EM densities using molecular dynamics - Pros and cons. *Journal of Structural Biology*, **2018**, 204, 319-328	3.4	6
196	Bacterial denitrifying nitric oxide reductases and aerobic respiratory terminal oxidases use similar delivery pathways for their molecular substrates. *Biochimica Et Biophysica Acta - Bioenergetics*, **2018**, 1859, 712-724	4.6	9
195	Menthol Stereoisomers Exhibit Different Effects on α2 nAChR Upregulation and Dopamine Neuron Spontaneous Firing. *ENeuro*, **2018**, 5,	3.9	9
194	The SERM/SERD bazedoxifene disrupts ESR1 helix 12 to overcome acquired hormone resistance in breast cancer cells. *ELife*, **2018**, 7,	8.9	42
193	Salt bridges gate β-catenin activation at intercellular junctions. *Molecular Biology of the Cell*, **2018**, 29, 111-122	3.5	12
192	Drug-Drug Interactions between Atorvastatin and Dronedarone Mediated by Monomeric CYP3A4. *Biochemistry*, **2018**, 57, 805-816	3.2	16
191	Calcium-Induced Lipid Nanocluster Structures: Sculpturing of the Plasma Membrane. *Biochemistry*, **2018**, 57, 6897-6905	3.2	9
190	Main-chain mutagenesis reveals intrahelical coupling in an ion channel voltage-sensor. *Nature Communications*, **2018**, 9, 5055	17.4	8
189	Endocannabinoid Virodhamine Is an Endogenous Inhibitor of Human Cardiovascular CYP2J2 Epoxygenase. *Biochemistry*, **2018**, 57, 6489-6499	3.2	11
188	Direct protein-lipid interactions shape the conformational landscape of secondary transporters. *Nature Communications*, **2018**, 9, 4151	17.4	70
187	Selective Permeability of Carboxysome Shell Pores to Anionic Molecules. *Journal of Physical Chemistry B*, **2018**, 122, 9110-9118	3.4	32

186	Structural basis of co-translational quality control by ArfA and RF2 bound to ribosome. *Nature*, **2017**, 541, 554-557	50.4	26
185	Mass spectrometry-based cross-linking study shows that the Psb28 protein binds to cytochrome in Photosystem II. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 2224-2229	11.5	25
184	A membrane-embedded pathway delivers general anesthetics to two interacting binding sites in the ion channel. *Journal of Biological Chemistry*, **2017**, 292, 9480-9492	5.4	15
183	Tribute to Klaus Schulten. *Journal of Physical Chemistry B*, **2017**, 121, 3203-3205	3.4	
182	Dimeric structure of the uracil:proton symporter UraA provides mechanistic insights into the SLC4/23/26 transporters. *Cell Research*, **2017**, 27, 1020-1033	24.7	59
181	Extension of the Highly Mobile Membrane Mimetic to Transmembrane Systems through Customized in Silico Solvents. *Journal of Physical Chemistry B*, **2017**, 121, 3764-3776	3.4	13
180	Energy transduction and alternating access of the mammalian ABC transporter P-glycoprotein. *Nature*, **2017**, 543, 738-741	50.4	141
179	Differential Membrane Binding Mechanics of Synaptotagmin Isoforms Observed in Atomic Detail. *Biochemistry*, **2017**, 56, 281-293	3.2	27
178	Chasing the open-state structure of pentameric ligand-gated ion channels. *Journal of General Physiology*, **2017**, 149, 1119-1138	3.4	25
177	Lipid specificity of the membrane binding domain of coagulation factor X. *Journal of Thrombosis and Haemostasis*, **2017**, 15, 2005-2016	15.4	17
176	Activation and Desensitization Mechanism of AMPA Receptor-TARP Complex by Cryo-EM. *Cell*, **2017**, 170, 1234-1246.e14	56.2	71
175	Arachidonic Acid Metabolism by Human Cardiovascular CYP2J2 Is Modulated by Doxorubicin. *Biochemistry*, **2017**, 56, 6700-6712	3.2	19
174	Critical Role of Water Molecules in Proton Translocation by the Membrane-Bound Transhydrogenase. *Structure*, **2017**, 25, 1111-1119.e3	5.2	8
173	Mitochondrial VDAC1: A Key Gatekeeper as Potential Therapeutic Target. *Frontiers in Physiology*, **2017**, 8, 460	4.6	139
172	Lipids and ions traverse the membrane by the same physical pathway in the nhTMEM16 scramblase. *ELife*, **2017**, 6,	8.9	64
171	Coupling X-Ray Reflectivity and In Silico Binding to Yield Dynamics of Membrane Recognition by Tim1. *Biophysical Journal*, **2017**, 113, 1505-1519	2.9	14
170	Microscopic Characterization of Membrane Transporter Function by In Silico Modeling and Simulation. *Methods in Enzymology*, **2016**, 578, 373-428	1.7	5
169	Asymmetric Binding and Metabolism of Polyunsaturated Fatty Acids (PUFAs) by CYP2J2 Epoxygenase. *Biochemistry*, **2016**, 55, 6969-6980	3.2	25

168	Q-Band Electron-Nuclear Double Resonance Reveals Out-of-Plane Hydrogen Bonds Stabilize an Anionic Ubisemiquinone in Cytochrome bo from Escherichia coli. *Biochemistry*, **2016**, 55, 5714-5725	3.2	8
167	X-ray structures define human P2X(3) receptor gating cycle and antagonist action. *Nature*, **2016**, 538, 66-71	50.4	134
166	Stapled Peptides with β-Methylated Hydrocarbon Chains for the Estrogen Receptor/Coactivator Interaction. *Angewandte Chemie*, **2016**, 128, 4324-4327	3.6	16
165	Molecular Basis for Differential Anion Binding and Proton Coupling in the Cl(-)/H(+) Exchanger ClC-ec1. *Journal of the American Chemical Society*, **2016**, 138, 3066-75	16.4	29
164	Enhancing Mn(II)-Binding and Manganese Peroxidase Activity in a Designed Cytochrome c Peroxidase through Fine-Tuning Secondary-Sphere Interactions. *Biochemistry*, **2016**, 55, 1494-502	3.2	15
163	All the O2 Consumed by Thermus thermophilus Cytochrome ba3 Is Delivered to the Active Site through a Long, Open Hydrophobic Tunnel with Entrances within the Lipid Bilayer. *Biochemistry*, **2016**, 55, 1265-78	3.2	15
162	Conformational Dynamics of the Human Islet Amyloid Polypeptide in a Membrane Environment: Toward the Aggregation Prone Form. *Biochemistry*, **2016**, 55, 2031-42	3.2	21
161	Revealing an outward-facing open conformational state in a CLC Cl(-)/H(+) exchange transporter. *ELife*, **2016**, 5,	8.9	31
160	Estrogen receptor alpha somatic mutations Y537S and D538G confer breast cancer endocrine resistance by stabilizing the activating function-2 binding conformation. *ELife*, **2016**, 5,	8.9	154
159	Stapled Peptides with β-Methylated Hydrocarbon Chains for the Estrogen Receptor/Coactivator Interaction. *Angewandte Chemie - International Edition*, **2016**, 55, 4252-5	16.4	62
158	The cellular membrane as a mediator for small molecule interaction with membrane proteins. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 2290-2304	3.8	30
157	TopoGromacs: Automated Topology Conversion from CHARMM to GROMACS within VMD. *Journal of Chemical Information and Modeling*, **2016**, 56, 1112-6	6.1	32
156	Atomic-level description of protein-lipid interactions using an accelerated membrane model. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1573-83	3.8	29
155	Binding Site Recognition and Docking Dynamics of a Single Electron Transport Protein: Cytochrome c2. *Journal of the American Chemical Society*, **2016**, 138, 12077-89	16.4	12
154	Incorporation of charged residues in the CYP2J2 F-G loop disrupts CYP2J2-lipid bilayer interactions. *Biochimica Et Biophysica Acta - Biomembranes*, **2015**, 1848, 2460-2470	3.8	30
153	Capturing Spontaneous Membrane Insertion of the Influenza Virus Hemagglutinin Fusion Peptide. *Journal of Physical Chemistry B*, **2015**, 119, 7882-93	3.4	30
152	Efficient Exploration of Membrane-Associated Phenomena at Atomic Resolution. *Journal of Membrane Biology*, **2015**, 248, 563-82	2.3	24
151	Redox potential tuning through differential quinone binding in the photosynthetic reaction center of Rhodobacter sphaeroides. *Biochemistry*, **2015**, 54, 2104-16	3.2	10

150	Computational characterization of structural dynamics underlying function in active membrane transporters. *Current Opinion in Structural Biology*, **2015**, 31, 96-105	8.1	41
149	Mechanism of drug-drug interactions mediated by human cytochrome P450 CYP3A4 monomer. *Biochemistry*, **2015**, 54, 2227-39	3.2	46
148	Atomic-level characterization of transport cycle thermodynamics in the glycerol-3-phosphate:phosphate antiporter. *Nature Communications*, **2015**, 6, 8393	17.4	66
147	Structural Determinants of the Mechanical Stability of □Catenin. *Journal of Biological Chemistry*, **2015**, 290, 18890-903	5.4	18
146	Membrane Interaction of the Factor VIIIa Discoidin Domains in Atomistic Detail. *Biochemistry*, **2015**, 54, 6123-31	3.2	13
145	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. *Biophysical Journal*, **2015**, 109, 2012-22	2.9	60
144	Visualizing Functional Motions of Membrane Transporters at an Atomic Resolution. *FASEB Journal*, **2015**, 29, 498.2	0.9	
143	Water access points and hydration pathways in CLC H+/Cl- transporters. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 1819-24	11.5	40
142	Changing the peptide specificity of a human T-cell receptor by directed evolution. *Nature Communications*, **2014**, 5, 5223	17.4	20
141	A highly tilted membrane configuration for the prefusion state of synaptobrevin. *Biophysical Journal*, **2014**, 107, 2112-21	2.9	28
140	Membrane-induced structural rearrangement and identification of a novel membrane anchor in talin F2F3. *Biophysical Journal*, **2014**, 107, 2059-69	2.9	31
139	Conformational heterogeneity of □synuclein in membrane. *Biochimica Et Biophysica Acta - Biomembranes*, **2014**, 1838, 3107-17	3.8	38
138	A microscopic view of phospholipid insertion into biological membranes. *Journal of Physical Chemistry B*, **2014**, 118, 1754-64	3.4	32
137	Conformational dynamics at the inner gate of KcsA during activation. *Biochemistry*, **2014**, 53, 2557-9	3.2	16
136	Atomistic models of general anesthetics for use in in silico biological studies. *Journal of Physical Chemistry B*, **2014**, 118, 12075-86	3.4	24
135	Computational Recipe for Efficient Description of Large-Scale Conformational Changes in Biomolecular Systems. *Journal of Chemical Theory and Computation*, **2014**, 10, 2866-2880	6.4	52
134	Partitioning of amino acids into a model membrane: capturing the interface. *Journal of Physical Chemistry B*, **2014**, 118, 1481-92	3.4	43
133	A Microscopic View of the Mechanisms of Active Transport Across the Cellular Membrane. *Annual Reports in Computational Chemistry*, **2014**, 10, 77-125	1.8	3

132	Conformational coupling between the active site and residues within the K(C)-channel of the Vibrio cholerae cbb3-type (C-family) oxygen reductase. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, E4419-28	11.5	7
131	Thermodynamic insight into spontaneous hydration and rapid water permeation in aquaporins. *Applied Physics Letters*, **2014**, 105, 083702	3.4	19
130	Molecular Dynamics: The Computational Molecular Microscope. *Razavi International Journal of Medicine*, **2014**, 2,		1
129	Conformational dynamics of the nucleotide binding domains and the power stroke of a heterodimeric ABC transporter. *ELife*, **2014**, 3, e02740	8.9	93
128	Rapid parameterization of small molecules using the Force Field Toolkit. *Journal of Computational Chemistry*, **2013**, 34, 2757-70	3.5	313
127	Characterizing a histidine switch controlling pH-dependent conformational changes of the influenza virus hemagglutinin. *Biophysical Journal*, **2013**, 105, 993-1003	2.9	16
126	Visualizing functional motions of membrane transporters with molecular dynamics simulations. *Biochemistry*, **2013**, 52, 569-87	3.2	39
125	Exploring Membrane-Bound form of the C2 Domain by HMMM Model. *Biophysical Journal*, **2013**, 104, 432a	2.9	2
124	Simulation studies of the mechanism of membrane transporters. *Methods in Molecular Biology*, **2013**, 924, 361-405	1.4	7
123	Driven Metadynamics: Reconstructing Equilibrium Free Energies from Driven Adaptive-Bias Simulations. *Journal of Physical Chemistry Letters*, **2013**, 4, 1882-1887	6.4	24
122	Characterizing the membrane-bound state of cytochrome P450 3A4: structure, depth of insertion, and orientation. *Journal of the American Chemical Society*, **2013**, 135, 8542-51	16.4	115
121	Subangstrom resolution X-ray structure details aquaporin-water interactions. *Science*, **2013**, 340, 1346-1349	33.3	147
120	Mechanistic picture for conformational transition of a membrane transporter at atomic resolution. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 18916-21	11.5	105
119	Movement of NH_3 through the human urea transporter B: a new gas channel. *American Journal of Physiology - Renal Physiology*, **2013**, 304, F1447-57	4.3	26
118	Transient formation of water-conducting states in membrane transporters. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 7696-701	11.5	72
117	On the origin of large flexibility of P-glycoprotein in the inward-facing state. *Journal of Biological Chemistry*, **2013**, 288, 19211-20	5.4	101
116	Tissue factor/factor VIIa complex: role of the membrane surface. *Thrombosis Research*, **2012**, 129 Suppl 2, S8-10	8.2	19
115	Molecular basis for the activation of a catalytic asparagine residue in a self-cleaving bacterial autotransporter. *Journal of Molecular Biology*, **2012**, 415, 128-42	6.5	34

114	A gate-free pathway for substrate release from the inward-facing state of the Na+-galactose transporter. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 263-71	3.8	21
113	Molecular dynamics investigation of the current in the Kv1.2 voltage sensor domains. *Biophysical Journal*, **2012**, 102, 258-67	2.9	38
112	Tracing cytoplasmic Ca(2+) ion and water access points in the Ca(2+)-ATPase. *Biophysical Journal*, **2012**, 102, 268-77	2.9	22
111	Accelerating membrane insertion of peripheral proteins with a novel membrane mimetic model. *Biophysical Journal*, **2012**, 102, 2130-9	2.9	98
110	Structure and permeation mechanism of a mammalian urea transporter. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 11194-9	11.5	58
109	Structural basis for iron piracy by pathogenic Neisseria. *Nature*, **2012**, 483, 53-8	50.4	199
108	Conformational coupling of the nucleotide-binding and the transmembrane domains in ABC transporters. *Biophysical Journal*, **2011**, 101, 680-90	2.9	43
107	Atomic view of calcium-induced clustering of phosphatidylserine in mixed lipid bilayers. *Biochemistry*, **2011**, 50, 2264-73	3.2	86
106	Nanoscale studies of protein-membrane interactions in blood clotting. *Journal of Thrombosis and Haemostasis*, **2011**, 9 Suppl 1, 162-7	15.4	22
105	Capturing spontaneous partitioning of peripheral proteins using a biphasic membrane-mimetic model. *Journal of Physical Chemistry B*, **2011**, 115, 7029-37	3.4	30
104	Membrane Transporters: Molecular Machines Coupling Cellular Energy to Vectorial Transport Across the Membrane **2011**, 151-181		
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