Emad Tajkhorshid

List of Publications by Citations

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	Scalable molecular dynamics with NAMD. *Journal of Computational Chemistry*, **2005**, 26, 1781-802	3.5	12650
274	Control of the selectivity of the aquaporin water channel family by global orientational tuning. *Science*, **2002**, 296, 525-30	33.3	742
273	Structural mechanism of plant aquaporin gating. *Nature*, **2006**, 439, 688-94	50.4	643
272	Free energy calculation from steered molecular dynamics simulations using Jarzynski equality. *Journal of Chemical Physics*, **2003**, 119, 3559-3566	3.9	600
271	Scalable molecular dynamics on CPU and GPU architectures with NAMD. *Journal of Chemical Physics* , **2020**, 153, 044130	3.9	483
270	Energetics of glycerol conduction through aquaglyceroporin GlpF. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 6731-6	11.5	334
269	Rapid parameterization of small molecules using the Force Field Toolkit. *Journal of Computational Chemistry*, **2013**, 34, 2757-70	3.5	313
268	Theory and simulation of water permeation in aquaporin-1. *Biophysical Journal*, **2004**, 86, 50-7	2.9	284
267	Pressure-induced water transport in membrane channels studied by molecular dynamics. *Biophysical Journal*, **2002**, 83, 154-60	2.9	252
266	Structural basis for iron piracy by pathogenic Neisseria. *Nature*, **2012**, 483, 53-8	50.4	199
265	Color tuning in rhodopsins: the mechanism for the spectral shift between bacteriorhodopsin and sensory rhodopsin II. *Journal of the American Chemical Society*, **2006**, 128, 10808-18	16.4	179
264	Collective diffusion model for water permeation through microscopic channels. *Physical Review Letters*, **2004**, 93, 224501	7.4	177
263	Molecular dynamics simulations of membrane channels and transporters. *Current Opinion in Structural Biology*, **2009**, 19, 128-37	8.1	174
262	Molecular dynamics simulations of proteins in lipid bilayers. *Current Opinion in Structural Biology*, **2005**, 15, 423-31	8.1	164
261	Molecular dynamics investigation of primary photoinduced events in the activation of rhodopsin. *Biophysical Journal*, **2002**, 83, 3097-112	2.9	163
260	Exploring gas permeability of cellular membranes and membrane channels with molecular dynamics. *Journal of Structural Biology*, **2007**, 157, 534-44	3.4	162
259	Classical force field parameters for the heme prosthetic group of cytochrome c. *Journal of Computational Chemistry*, **2004**, 25, 1613-22	3.5	161

258	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
257	Electrostatic tuning of permeation and selectivity in aquaporin water channels. *Biophysical Journal*, **2003**, 85, 2884-99	2.9	150
256	Subangstrom resolution X-ray structure details aquaporin-water interactions. *Science*, **2013**, 340, 1346-1349	33.3	147
255	What makes an aquaporin a glycerol channel? A comparative study of AqpZ and GlpF. *Structure*, **2005**, 13, 1107-18	5.2	147
254	Structure of the alternative complex III in a supercomplex with cytochrome oxidase. *Nature*, **2018**, 557, 123-126	50.4	144
253	Energy transduction and alternating access of the mammalian ABC transporter P-glycoprotein. *Nature*, **2017**, 543, 738-741	50.4	141
252	Mitochondrial VDAC1: A Key Gatekeeper as Potential Therapeutic Target. *Frontiers in Physiology*, **2017**, 8, 460	4.6	139
251	The mechanism of glycerol conduction in aquaglyceroporins. *Structure*, **2001**, 9, 1083-93	5.2	139
250	The mechanism of proton exclusion in aquaporin channels. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 223-8	4.2	136
249	X-ray structures define human P2X(3) receptor gating cycle and antagonist action. *Nature*, **2016**, 538, 66-71	50.4	134
248	Molecular basis of proton blockage in aquaporins. *Structure*, **2004**, 12, 65-74	5.2	132
247	Mechanism of gating and ion conductivity of a possible tetrameric pore in aquaporin-1. *Structure*, **2006**, 14, 1411-23	5.2	126
246	Molecular dynamics simulation of bacteriorhodopsin's photoisomerization using ab initio forces for the excited chromophore. *Biophysical Journal*, **2003**, 85, 1440-9	2.9	126
245	Structural changes during the formation of early intermediates in the bacteriorhodopsin photocycle. *Biophysical Journal*, **2002**, 83, 1281-97	2.9	124
244	Calculation of the gating charge for the Kv1.2 voltage-activated potassium channel. *Biophysical Journal*, **2010**, 98, 2189-98	2.9	121
243	Unique conformer selection of human growth-regulatory lectin galectin-1 for ganglioside GM1 versus bacterial toxins. *Biochemistry*, **2003**, 42, 14762-73	3.2	116
242	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
241	Peptide aggregation and pore formation in a lipid bilayer: a combined coarse-grained and all atom molecular dynamics study. *Biophysical Journal*, **2008**, 95, 4337-47	2.9	113

240	Electrostatic funneling of substrate in mitochondrial inner membrane carriers. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 9598-603	11.5	110
239	Structural Determinants of Spectral Tuning in Retinal ProteinsBacteriorhodopsin vs Sensory Rhodopsin II#. *Journal of Physical Chemistry B*, **2001**, 105, 10124-10131	3.4	106
238	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
237	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
236	Functional interplay between acetylation and methylation of the RelA subunit of NF-kappaB. *Molecular and Cellular Biology*, **2010**, 30, 2170-80	4.8	101
235	Accelerating membrane insertion of peripheral proteins with a novel membrane mimetic model. *Biophysical Journal*, **2012**, 102, 2130-9	2.9	98
234	Photochemical reaction dynamics of the primary event of vision studied by means of a hybrid molecular simulation. *Biophysical Journal*, **2009**, 96, 403-16	2.9	98
233	Dynamics of K+ ion conduction through Kv1.2. *Biophysical Journal*, **2006**, 91, L72-4	2.9	98
232	Molecular dynamics study of the nature and origin of retinal's twisted structure in bacteriorhodopsin. *Biophysical Journal*, **2000**, 78, 683-93	2.9	95
231	Conformational dynamics of the nucleotide binding domains and the power stroke of a heterodimeric ABC transporter. *ELife*, **2014**, 3, e02740	8.9	93
230	Serotonin transporter-ibogaine complexes illuminate mechanisms of inhibition and transport. *Nature*, **2019**, 569, 141-145	50.4	89
229	Mechanics of force propagation in TonB-dependent outer membrane transport. *Biophysical Journal*, **2007**, 93, 496-504	2.9	88
228	Diffusion of glycerol through Escherichia coli aquaglyceroporin GlpF. *Biophysical Journal*, **2008**, 94, 832-9	2.9	87
227	Substrate binding and formation of an occluded state in the leucine transporter. *Biophysical Journal* , **2008**, 94, 1600-12	2.9	87
226	Atomic view of calcium-induced clustering of phosphatidylserine in mixed lipid bilayers. *Biochemistry*, **2011**, 50, 2264-73	3.2	86
225	Mechanisms of selectivity in channels and enzymes studied with interactive molecular dynamics. *Biophysical Journal*, **2003**, 85, 36-48	2.9	86
224	Molecular Dynamics Study of Bacteriorhodopsin and the Purple Membrane. *Journal of Physical Chemistry B*, **2001**, 105, 905-918	3.4	86
223	Structural and functional analysis of SoPIP2;1 mutants adds insight into plant aquaporin gating. *Journal of Molecular Biology*, **2009**, 387, 653-68	6.5	82

222	Toward theoretical analysis of long-range proton transfer kinetics in biomolecular pumps. *Journal of Physical Chemistry A*, **2006**, 110, 548-63	2.8	82
221	Molecular dynamics study of aquaporin-1 water channel in a lipid bilayer. *FEBS Letters*, **2001**, 504, 212-8	3.8	81
220	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
219	Determination of structural and functional overlap/divergence of five proto-type galectins by analysis of the growth-regulatory interaction with ganglioside GM1 in silico and in vitro on human neuroblastoma cells. *International Journal of Cancer*, **2005**, 114, 46-57	7.5	79
218	A comparison of aqueous solvent models used in the calculation of the Raman and ROA spectra of l-alanine. *Chemical Physics*, **2001**, 265, 125-151	2.3	79
217	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
216	Molecular determinants of phospholipid synergy in blood clotting. *Journal of Biological Chemistry*, **2011**, 286, 23247-53	5.4	76
215	Performance of the AM1, PM3, and SCC-DFTB methods in the study of conjugated Schiff base molecules. *Chemical Physics*, **2002**, 277, 91-103	2.3	74
214	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
213	Activation and Desensitization Mechanism of AMPA Receptor-TARP Complex by Cryo-EM. *Cell*, **2017**, 170, 1234-1246.e14	56.2	71
212	Dynamics of the extracellular gate and ion-substrate coupling in the glutamate transporter. *Biophysical Journal*, **2008**, 95, 2292-300	2.9	71
211	Direct protein-lipid interactions shape the conformational landscape of secondary transporters. *Nature Communications*, **2018**, 9, 4151	17.4	70
210	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. *Cell*, **2019**, 179, 1098-1111.e23	36.1	67
209	Dimer opening of the nucleotide binding domains of ABC transporters after ATP hydrolysis. *Biophysical Journal*, **2008**, 95, 5100-10	2.9	67
208	Atomic-level characterization of transport cycle thermodynamics in the glycerol-3-phosphate:phosphate antiporter. *Nature Communications*, **2015**, 6, 8393	17.4	66
207	Mechanism of signal propagation upon retinal isomerization: insights from molecular dynamics simulations of rhodopsin restrained by normal modes. *Biophysical Journal*, **2008**, 95, 789-803	2.9	66
206	Structural and functional diversity calls for a new classification of ABC transporters. *FEBS Letters*, **2020**, 594, 3767-3775	3.8	66
205	Lipids and ions traverse the membrane by the same physical pathway in the nhTMEM16 scramblase. *ELife*, **2017**, 6,	8.9	64

204	Modeling and dynamics of the inward-facing state of a Na+/Cl- dependent neurotransmitter transporter homologue. *PLoS Computational Biology*, **2010**, 6, e1000905	5	63
203	Nitric oxide conduction by the brain aquaporin AQP4. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 661-70	4.2	63
202	Sugar transport across lactose permease probed by steered molecular dynamics. *Biophysical Journal*, **2007**, 93, 92-102	2.9	62
201	Role of hydrogen-bond network in energy storage of bacteriorhodopsin's light-driven proton pump revealed by ab initio normal-mode analysis. *Journal of the American Chemical Society*, **2004**, 126, 10516-7	16.4	62
200	Stapled Peptides with α-Methylated Hydrocarbon Chains for the Estrogen Receptor/Coactivator Interaction. *Angewandte Chemie - International Edition*, **2016**, 55, 4252-5	16.4	62
199	Identification of the third Na+ site and the sequence of extracellular binding events in the glutamate transporter. *Biophysical Journal*, **2010**, 99, 1416-25	2.9	61
198	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. *Biophysical Journal*, **2015**, 109, 2012-22	2.9	60
197	Incorporation of antimicrobial peptides into membranes: a combined liquid-state NMR and molecular dynamics study of alamethicin in DMPC/DHPC bicelles. *Journal of Physical Chemistry B*, **2009**, 113, 6928-37	3.4	60
196	Distinct structural and adhesive roles of Ca2+ in membrane binding of blood coagulation factors. *Structure*, **2008**, 16, 72-81	5.2	60
195	Molecular mechanisms of conduction and selectivity in aquaporin water channels. *Journal of Nutrition*, **2007**, 137, 1509S-1515S; discussion 1516S-1517S	4.1	60
194	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
193	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
192	Lectin ligands: new insights into their conformations and their dynamic behavior and the discovery of conformer selection by lectins. *Cells Tissues Organs*, **1998**, 161, 91-109	2.1	56
191	Sugar binding and protein conformational changes in lactose permease. *Biophysical Journal*, **2006**, 91, 3972-85	2.9	55
190	Ion-releasing state of a secondary membrane transporter. *Biophysical Journal*, **2009**, 97, L29-31	2.9	54
189	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
188	Tyrosine phosphorylation by Src within the cavity of the adenine nucleotide translocase 1 regulates ADP/ATP exchange in mitochondria. *American Journal of Physiology - Cell Physiology*, **2010**, 298, C740-8	5.4	49
187	Involvement of laser photo-CIDNP (chemically induced dynamic nuclear polarization)-reactive amino acid side chains in ligand binding by galactoside-specific lectins in solution. *FEBS Journal*, **1997**, 249, 27-38		48

186	Developing an energy landscape for the novel function of a (beta/alpha)8 barrel: ammonia conduction through HisF. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 7599-604	11.5	48
185	Mechanism of drug-drug interactions mediated by human cytochrome P450 CYP3A4 monomer. *Biochemistry*, **2015**, 54, 2227-39	3.2	46
184	Partitioning of amino acids into a model membrane: capturing the interface. *Journal of Physical Chemistry B*, **2014**, 118, 1481-92	3.4	43
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181	The SERM/SERD bazedoxifene disrupts ESR1 helix 12 to overcome acquired hormone resistance in breast cancer cells. *ELife*, **2018**, 7,	8.9	42
180	Computational characterization of structural dynamics underlying function in active membrane transporters. *Current Opinion in Structural Biology*, **2015**, 31, 96-105	8.1	41
179	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
178	PyContact: Rapid, Customizable, and Visual Analysis of Noncovalent Interactions in MD Simulations. *Biophysical Journal*, **2018**, 114, 577-583	2.9	39
177	Visualizing functional motions of membrane transporters with molecular dynamics simulations. *Biochemistry*, **2013**, 52, 569-87	3.2	39
176	Conformational heterogeneity of □synuclein in membrane. *Biochimica Et Biophysica Acta - Biomembranes*, **2014**, 1838, 3107-17	3.8	38
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174	Exploring transmembrane diffusion pathways with molecular dynamics. *Physiology*, **2010**, 25, 142-54	9.8	38
173	Structural basis of substrate selectivity in the glycerol-3-phosphate: phosphate antiporter GlpT. *Biophysical Journal*, **2009**, 97, 1346-53	2.9	35
172	Blood clotting reactions on nanoscale phospholipid bilayers. *Thrombosis Research*, **2008**, 122 Suppl 1, S23-6	8.2	35
171	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
170	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
169	Simulation of spontaneous substrate binding revealing the binding pathway and mechanism and initial conformational response of GlpT. *Biochemistry*, **2010**, 49, 1105-14	3.2	33

168	A microscopic view of phospholipid insertion into biological membranes. *Journal of Physical Chemistry B*, **2014**, 118, 1754-64	3.4	32
167	Residue-specific information about the dynamics of antimicrobial peptides from (1)H-(15)N and (2)H solid-state NMR spectroscopy. *Journal of the American Chemical Society*, **2009**, 131, 18335-42	16.4	32
166	TopoGromacs: Automated Topology Conversion from CHARMM to GROMACS within VMD. *Journal of Chemical Information and Modeling*, **2016**, 56, 1112-6	6.1	32
165	Selective Permeability of Carboxysome Shell Pores to Anionic Molecules. *Journal of Physical Chemistry B*, **2018**, 122, 9110-9118	3.4	32
164	Membrane-induced structural rearrangement and identification of a novel membrane anchor in talin F2F3. *Biophysical Journal*, **2014**, 107, 2059-69	2.9	31
163	The binding interface of cytochrome c and cytochrome c in the bc complex: rationalizing the role of key residues. *Biophysical Journal*, **2010**, 99, 2647-56	2.9	31
162	Role of Water in Transient Cytochrome c2Docking. *Journal of Physical Chemistry B*, **2004**, 108, 20376-20387	3.4	31
161	Revealing an outward-facing open conformational state in a CLC Cl(-)/H(+) exchange transporter. *ELife*, **2016**, 5,	8.9	31
160	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
159	Structural insights into photosystem II assembly. *Nature Plants*, **2021**, 7, 524-538	11.5	31
158	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
157	Capturing Spontaneous Membrane Insertion of the Influenza Virus Hemagglutinin Fusion Peptide. *Journal of Physical Chemistry B*, **2015**, 119, 7882-93	3.4	30
156	A Chalcogen-Bonding Cascade Switch for Planarizable Push-Pull Probes. *Angewandte Chemie - International Edition*, **2019**, 58, 15752-15756	16.4	30
155	Capturing spontaneous partitioning of peripheral proteins using a biphasic membrane-mimetic model. *Journal of Physical Chemistry B*, **2011**, 115, 7029-37	3.4	30
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152	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
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150	Atomic-level description of protein-lipid interactions using an accelerated membrane model. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1573-83	3.8	29
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148	Differential Membrane Binding Mechanics of Synaptotagmin Isoforms Observed in Atomic Detail. *Biochemistry*, **2017**, 56, 281-293	3.2	27
147	Coupling of calcium and substrate binding through loop alignment in the outer-membrane transporter BtuB. *Journal of Molecular Biology*, **2009**, 393, 1129-42	6.5	27
146	Structural basis of co-translational quality control by ArfA and RF2 bound to ribosome. *Nature*, **2017**, 541, 554-557	50.4	26
145	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
144	Movement of NH□through the human urea transporter B: a new gas channel. *American Journal of Physiology - Renal Physiology*, **2013**, 304, F1447-57	4.3	26
143	Potential cation and H+ binding sites in acid sensing ion channel-1. *Biophysical Journal*, **2008**, 95, 5153-64	2.9	26
142	Tuning symmetry breaking charge separation in perylene bichromophores by conformational control. *Chemical Science*, **2019**, 10, 10629-10639	9.4	26
141	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
140	Chasing the open-state structure of pentameric ligand-gated ion channels. *Journal of General Physiology*, **2017**, 149, 1119-1138	3.4	25
139	Asymmetric Binding and Metabolism of Polyunsaturated Fatty Acids (PUFAs) by CYP2J2 Epoxygenase. *Biochemistry*, **2016**, 55, 6969-6980	3.2	25
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137	Atomistic models of general anesthetics for use in in silico biological studies. *Journal of Physical Chemistry B*, **2014**, 118, 12075-86	3.4	24
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130	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
129	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
128	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
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125	A "cross-stitched" peptide with improved helicity and proteolytic stability. *Organic and Biomolecular Chemistry*, **2018**, 16, 3702-3706	3.9	19
124	Arachidonic Acid Metabolism by Human Cardiovascular CYP2J2 Is Modulated by Doxorubicin. *Biochemistry*, **2017**, 56, 6700-6712	3.2	19
123	Thermodynamic insight into spontaneous hydration and rapid water permeation in aquaporins. *Applied Physics Letters*, **2014**, 105, 083702	3.4	19
122	Tissue factor/factor VIIa complex: role of the membrane surface. *Thrombosis Research*, **2012**, 129 Suppl 2, S8-10	8.2	19
121	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
120	Structural Determinants of the Mechanical Stability of □Catenin. *Journal of Biological Chemistry*, **2015**, 290, 18890-903	5.4	18
119	Identifying mutation hotspots reveals pathogenetic mechanisms of KCNQ2 epileptic encephalopathy. *Scientific Reports*, **2020**, 10, 4756	4.9	18
118	Structural basis for the reaction cycle of DASS dicarboxylate transporters. *ELife*, **2020**, 9,	8.9	18
117	Microscopic view of lipids and their diverse biological functions. *Current Opinion in Structural Biology*, **2018**, 51, 177-186	8.1	17
116	Lipid specificity of the membrane binding domain of coagulation factor X. *Journal of Thrombosis and Haemostasis*, **2017**, 15, 2005-2016	15.4	17
115	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

114	Microscopic Characterization of GRP1 PH Domain Interaction with Anionic Membranes. *Journal of Computational Chemistry*, **2020**, 41, 489-499	3.5	16
113	Stapled Peptides with α-Methylated Hydrocarbon Chains for the Estrogen Receptor/Coactivator Interaction. *Angewandte Chemie*, **2016**, 128, 4324-4327	3.6	16
112	Conformational dynamics at the inner gate of KcsA during activation. *Biochemistry*, **2014**, 53, 2557-9	3.2	16
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110	Resolution enhancement in solid-state NMR of oriented membrane proteins by anisotropic differential linebroadening. *Journal of the American Chemical Society*, **2008**, 130, 5028-9	16.4	16
109	Boosting Free-Energy Perturbation Calculations with GPU-Accelerated NAMD. *Journal of Chemical Information and Modeling*, **2020**, 60, 5301-5307	6.1	16
108	Drug-Drug Interactions between Atorvastatin and Dronedarone Mediated by Monomeric CYP3A4. *Biochemistry*, **2018**, 57, 805-816	3.2	16
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106	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
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