

Rainer Arnold Bckmann

List of Publications by Citations

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74
papers

4,543
citations

31
h-index

67
g-index

81
ext. papers

5,420
ext. citations

4.7
avg, IF

5.82
L-index

#	Paper	IF	Citations
74	Computational Lipidomics with insane: A Versatile Tool for Generating Custom Membranes for Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2144-55	6.4	504
73	Effect of sodium chloride on a lipid bilayer. <i>Biophysical Journal</i> , 2003 , 85, 1647-55	2.9	452
72	Going Backward: A Flexible Geometric Approach to Reverse Transformation from Coarse Grained to Atomistic Models. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 676-90	6.4	378
71	Optimization of the OPLS-AA Force Field for Long Hydrocarbons. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1459-70	6.4	364
70	Kinetics, statistics, and energetics of lipid membrane electroporation studied by molecular dynamics simulations. <i>Biophysical Journal</i> , 2008 , 95, 1837-50	2.9	230
69	Biomolecular simulations of membranes: physical properties from different force fields. <i>Journal of Chemical Physics</i> , 2008 , 128, 125103	3.9	227
68	Predicting free energy changes using structural ensembles. <i>Nature Methods</i> , 2009 , 6, 3-4	21.6	196
67	Multistep binding of divalent cations to phospholipid bilayers: a molecular dynamics study. <i>Angewandte Chemie - International Edition</i> , 2004 , 43, 1021-4	16.4	164
66	The closure of Pak1-dependent macropinosomes requires the phosphorylation of CtBP1/BARS. <i>EMBO Journal</i> , 2008 , 27, 970-81	13	147
65	Effects of alkali cations and halide anions on the DOPC lipid membrane. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 7235-43	2.8	133
64	The Multifaceted Role of SNARE Proteins in Membrane Fusion. <i>Frontiers in Physiology</i> , 2017 , 8, 5	4.6	121
63	A Critical Comparison of Biomembrane Force Fields: Structure and Dynamics of Model DMPC, POPC, and POPE Bilayers. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 3888-903	3.4	95
62	Mechanism of interaction of monovalent ions with phosphatidylcholine lipid membranes. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 9504-9	3.4	81
61	Differential peptide dynamics is linked to major histocompatibility complex polymorphism. <i>Journal of Biological Chemistry</i> , 2004 , 279, 28197-201	5.4	74
60	High-Throughput Simulations of Dimer and Trimer Assembly of Membrane Proteins. The DAFT Approach. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2278-91	6.4	73
59	Membrane-Mediated Oligomerization of G Protein Coupled Receptors and Its Implications for GPCR Function. <i>Frontiers in Physiology</i> , 2016 , 7, 494	4.6	72
58	Nanoseconds molecular dynamics simulation of primary mechanical energy transfer steps in F1-ATP synthase. <i>Nature Structural Biology</i> , 2002 , 9, 198-202		64

57	Dynamic Cholesterol-Conditioned Dimerization of the G Protein Coupled Chemokine Receptor Type 4. <i>PLoS Computational Biology</i> , 2016 , 12, e1005169	5	61
56	Dynamical characterization of two differentially disease associated MHC class I proteins in complex with viral and self-peptides. <i>Journal of Molecular Biology</i> , 2012 , 415, 429-42	6.5	60
55	1-Alkanols and membranes: a story of attraction. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2007 , 1768, 2899-913	3.8	55
54	Biomembranes in atomistic and coarse-grained simulations. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 323103	1.8	50
53	HLA-B27 subtypes differentially associated with disease exhibit conformational differences in solution. <i>Journal of Molecular Biology</i> , 2008 , 376, 798-810	6.5	50
52	Spontaneous formation of detergent micelles around the outer membrane protein OmpX. <i>Biophysical Journal</i> , 2005 , 88, 3191-204	2.9	48
51	The influence of 1-alkanols and external pressure on the lateral pressure profiles of lipid bilayers. <i>Biophysical Journal</i> , 2008 , 95, 5766-78	2.9	47
50	Critical Comparison of Biomembrane Force Fields: Protein-Lipid Interactions at the Membrane Interface. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 2310-2321	6.4	42
49	Membrane pore formation in atomistic and coarse-grained simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016 , 1858, 2266-2277	3.8	41
48	Conformational dynamics of the F1-ATPase beta-subunit: a molecular dynamics study. <i>Biophysical Journal</i> , 2003 , 85, 1482-91	2.9	38
47	v-SNARE transmembrane domains function as catalysts for vesicle fusion. <i>ELife</i> , 2016 , 5,	8.9	36
46	Electric field effects on membranes: gramicidin A as a test ground. <i>Journal of Structural Biology</i> , 2007 , 157, 545-56	3.4	34
45	High-resolution structures of Escherichia coli cDsbD in different redox states: A combined crystallographic, biochemical and computational study. <i>Journal of Molecular Biology</i> , 2006 , 358, 829-45	6.5	34
44	HLA-B27 and antigen presentation: at the crossroads between immune defense and autoimmunity. <i>Molecular Immunology</i> , 2014 , 57, 22-7	4.3	33
43	Low-affinity peptides and T-cell selection. <i>Trends in Immunology</i> , 2009 , 30, 53-60	14.4	29
42	Membrane-proximal tryptophans of synaptobrevin II stabilize priming of secretory vesicles. <i>Journal of Neuroscience</i> , 2012 , 32, 15983-97	6.6	28
41	Extension of the LOPLS-AA Force Field for Alcohols, Esters, and Monoolein Bilayers and its Validation by Neutron Scattering Experiments. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 15287-99	3.4	25
40	A Coiled-Coil Peptide Shaping Lipid Bilayers upon Fusion. <i>Biophysical Journal</i> , 2016 , 111, 2162-2175	2.9	25

39	Spontaneous adsorption of coiled-coil model peptides K and E to a mixed lipid bilayer. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 4396-408	3.4	24
38	Closely related, yet unique: Distinct homo- and heterodimerization patterns of G protein coupled chemokine receptors and their fine-tuning by cholesterol. <i>PLoS Computational Biology</i> , 2018 , 14, e1006062	5.2	24
37	Synaptobrevin transmembrane domain determines the structure and dynamics of the SNARE motif and the linker region. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016 , 1858, 855-65	3.8	22
36	The function of the two-pore channel TPC1 depends on dimerization of its carboxy-terminal helix. <i>Cellular and Molecular Life Sciences</i> , 2016 , 73, 2565-81	10.3	20
35	Molecular dynamics simulations of membrane proteins. <i>Methods in Molecular Biology</i> , 2013 , 1033, 85-101	1.4	19
34	Phosphatidylinositol-3,5-bisphosphate lipid-binding-induced activation of the human two-pore channel 2. <i>Cellular and Molecular Life Sciences</i> , 2018 , 75, 3803-3815	10.3	18
33	Synaptobrevin Transmembrane Domain Dimerization Studied by Multiscale Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2015 , 109, 760-71	2.9	17
32	Binding Characteristics of Sphingosine-1-Phosphate to ApoM hints to Assisted Release Mechanism via the ApoM Calyx-Opening. <i>Scientific Reports</i> , 2016 , 6, 30655	4.9	17
31	Molecular determinants of major histocompatibility complex class I complex stability: shaping antigenic features through short and long range electrostatic interactions. <i>Journal of Biological Chemistry</i> , 2008 , 283, 23093-103	5.4	17
30	Generation of antimicrobial peptides Leg1 and Leg2 from chickpea storage protein, active against food spoilage bacteria and foodborne pathogens. <i>Food Chemistry</i> , 2021 , 347, 128917	8.5	17
29	Membrane phase transition during heating and cooling: molecular insight into reversible melting. <i>European Biophysics Journal</i> , 2018 , 47, 151-164	1.9	16
28	Coupling of Membrane Nanodomain Formation and Enhanced Electroporation near Phase Transition. <i>Biophysical Journal</i> , 2019 , 116, 2131-2148	2.9	15
27	Interaction pattern of Arg 62 in the A-pocket of differentially disease-associated HLA-B27 subtypes suggests distinct TCR binding modes. <i>PLoS ONE</i> , 2012 , 7, e32865	3.7	14
26	Crystal Structures of the Global Regulator DasR from <i>Streptomyces coelicolor</i> : Implications for the Allosteric Regulation of GntR/HutC Repressors. <i>PLoS ONE</i> , 2016 , 11, e0157691	3.7	14
25	Dynamic processes in biological membrane mimics revealed by quasielastic neutron scattering. <i>Chemistry and Physics of Lipids</i> , 2017 , 206, 28-42	3.7	13
24	Low free energy barrier for ion permeation through double-helical gramicidin. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 3195-202	3.4	13
23	Oxidative Stress-Induced STIM2 Cysteine Modifications Suppress Store-Operated Calcium Entry. <i>Cell Reports</i> , 2020 , 33, 108292	10.6	12
22	Phase Transition of Glycolipid Membranes Studied by Coarse-Grained Simulations. <i>Langmuir</i> , 2015 , 31, 9379-87	4	11

21	Energetic view on membrane pore formation. <i>Biophysical Journal</i> , 2014 , 106, 1-2	2.9	11
20	Exploring the Formation and the Structure of Synaptobrevin Oligomers in a Model Membrane. <i>Biophysical Journal</i> , 2016 , 110, 2004-15	2.9	11
19	Peptide-induced membrane curvature in edge-stabilized open bilayers: a theoretical and molecular dynamics study. <i>Journal of Chemical Physics</i> , 2014 , 141, 024901	3.9	10
18	Characteristics of Sucrose Transport through the Sucrose-Specific Porin ScrY Studied by Molecular Dynamics Simulations. <i>Frontiers in Bioengineering and Biotechnology</i> , 2016 , 4, 9	5.8	10
17	Comprehensive Characterization of Lipid-Guided G Protein-Coupled Receptor Dimerization. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 2823-2834	3.4	9
16	Contribution of charged and polar residues for the formation of the E1-E2 heterodimer from Hepatitis C Virus. <i>Journal of Molecular Modeling</i> , 2010 , 16, 1625-37	2	9
15	Evidence for proton shuffling in a thioredoxin-like protein during catalysis. <i>Journal of Molecular Biology</i> , 2008 , 382, 978-86	6.5	9
14	The Molecular Switching Mechanism at the Conserved D(E)RY Motif in Class-A GPCRs. <i>Biophysical Journal</i> , 2016 , 111, 79-89	2.9	9
13	Structural Model of the mIgM B-Cell Receptor Transmembrane Domain From Self-Association Molecular Dynamics Simulations. <i>Frontiers in Immunology</i> , 2018 , 9, 2947	8.4	8
12	Maturation of Monocyte-Derived DCs Leads to Increased Cellular Stiffness, Higher Membrane Fluidity, and Changed Lipid Composition. <i>Frontiers in Immunology</i> , 2020 , 11, 590121	8.4	7
11	Serotonin Alters the Phase Equilibrium of a Ternary Mixture of Phospholipids and Cholesterol. <i>Frontiers in Physiology</i> , 2020 , 11, 578868	4.6	6
10	The degenerin region of the human bile acid-sensitive ion channel (BASIC) is involved in channel inhibition by calcium and activation by bile acids. <i>Pflugers Archiv European Journal of Physiology</i> , 2018 , 470, 1087-1102	4.6	5
9	Allostery in BAX protein activation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016 , 34, 2469-80	3.6	5
8	Spontaneous Membrane Nanodomain Formation in the Absence or Presence of the Neurotransmitter Serotonin. <i>Frontiers in Cell and Developmental Biology</i> , 2020 , 8, 601145	5.7	4
7	Lipid Dynamics in Membranes Slowed Down by Transmembrane Proteins. <i>Frontiers in Cell and Developmental Biology</i> , 2020 , 8, 579388	5.7	4
6	Molekulare Nanomaschinen unter der Lupe: Proteindynamik-Simulationen. <i>Physik in Unserer Zeit</i> , 2006 , 37, 73-79	0.1	3
5	Drug-Induced Dynamics of Bile Colloids. <i>Langmuir</i> , 2021 , 37, 2543-2551	4	3
4	GroPBS: Fast Solver for Implicit Electrostatics of Biomolecules. <i>Frontiers in Bioengineering and Biotechnology</i> , 2015 , 3, 186	5.8	2

- 3 Going Backward: An Efficient Multiscale Approach using Reverse Transformation. *Biophysical Journal*, **2014**, 106, 640a 2.9 2
- 2 Molecular dynamics simulation of lipids and lipid embossed proteins. *Chemistry and Physics of Lipids*, **2007**, 149, S4 3.7
- 1 Cover Picture: Multistep Binding of Divalent Cations to Phospholipid Bilayers: A Molecular Dynamics Study (Angew. Chem. Int. Ed. 8/2004). *Angewandte Chemie - International Edition*, **2004**, 43, 911-911 16.4