Rainer Arnold Bckmann

List of Publications by Year in Descending Order

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	Generation of antimicrobial peptides Leg1 and Leg2 from chickpea storage protein, active against food spoilage bacteria and foodborne pathogens. *Food Chemistry*, **2021**, 347, 128917	8.5	17
73	Drug-Induced Dynamics of Bile Colloids. *Langmuir*, **2021**, 37, 2543-2551	4	3
72	Spontaneous Membrane Nanodomain Formation in the Absence or Presence of the Neurotransmitter Serotonin. *Frontiers in Cell and Developmental Biology*, **2020**, 8, 601145	5.7	4
71	Comprehensive Characterization of Lipid-Guided G Protein-Coupled Receptor Dimerization. *Journal of Physical Chemistry B*, **2020**, 124, 2823-2834	3.4	9
70	Oxidative Stress-Induced STIM2 Cysteine Modifications Suppress Store-Operated Calcium Entry. *Cell Reports*, **2020**, 33, 108292	10.6	12
69	Lipid Dynamics in Membranes Slowed Down by Transmembrane Proteins. *Frontiers in Cell and Developmental Biology*, **2020**, 8, 579388	5.7	4
68	Serotonin Alters the Phase Equilibrium of a Ternary Mixture of Phospholipids and Cholesterol. *Frontiers in Physiology*, **2020**, 11, 578868	4.6	6
67	Maturation of Monocyte-Derived DCs Leads to Increased Cellular Stiffness, Higher Membrane Fluidity, and Changed Lipid Composition. *Frontiers in Immunology*, **2020**, 11, 590121	8.4	7
66	Coupling of Membrane Nanodomain Formation and Enhanced Electroporation near Phase Transition. *Biophysical Journal*, **2019**, 116, 2131-2148	2.9	15
65	The degenerin region of the human bile acid-sensitive ion channel (BASIC) is involved in channel inhibition by calcium and activation by bile acids. *Pflugers Archiv European Journal of Physiology*, **2018**, 470, 1087-1102	4.6	5
64	Phosphatidylinositol-3,5-bisphosphate lipid-binding-induced activation of the human two-pore channel 2. *Cellular and Molecular Life Sciences*, **2018**, 75, 3803-3815	10.3	18
63	Closely related, yet unique: Distinct homo- and heterodimerization patterns of G protein coupled chemokine receptors and their fine-tuning by cholesterol. *PLoS Computational Biology*, **2018**, 14, e1006062	5	24
62	Membrane phase transition during heating and cooling: molecular insight into reversible melting. *European Biophysics Journal*, **2018**, 47, 151-164	1.9	16
61	Structural Model of the mIgM B-Cell Receptor Transmembrane Domain From Self-Association Molecular Dynamics Simulations. *Frontiers in Immunology*, **2018**, 9, 2947	8.4	8
60	Dynamic processes in biological membrane mimics revealed by quasielastic neutron scattering. *Chemistry and Physics of Lipids*, **2017**, 206, 28-42	3.7	13
59	Critical Comparison of Biomembrane Force Fields: Protein-Lipid Interactions at the Membrane Interface. *Journal of Chemical Theory and Computation*, **2017**, 13, 2310-2321	6.4	42
58	The Multifaceted Role of SNARE Proteins in Membrane Fusion. *Frontiers in Physiology*, **2017**, 8, 5	4.6	121

57	Binding Characteristics of Sphingosine-1-Phosphate to ApoM hints to Assisted Release Mechanism via the ApoM Calyx-Opening. *Scientific Reports*, **2016**, 6, 30655	4.9	17
56	A Coiled-Coil Peptide Shaping Lipid Bilayers upon Fusion. *Biophysical Journal*, **2016**, 111, 2162-2175	2.9	25
55	Synaptobrevin transmembrane domain determines the structure and dynamics of the SNARE motif and the linker region. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 855-65	3.8	22
54	Allostery in BAX protein activation. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 2469-80	3.6	5
53	Membrane pore formation in atomistic and coarse-grained simulations. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 2266-2277	3.8	41
52	Dynamic Cholesterol-Conditioned Dimerization of the G Protein Coupled Chemokine Receptor Type 4. *PLoS Computational Biology*, **2016**, 12, e1005169	5	61
51	v-SNARE transmembrane domains function as catalysts for vesicle fusion. *ELife*, **2016**, 5,	8.9	36
50	Characteristics of Sucrose Transport through the Sucrose-Specific Porin ScrY Studied by Molecular Dynamics Simulations. *Frontiers in Bioengineering and Biotechnology*, **2016**, 4, 9	5.8	10
49	Crystal Structures of the Global Regulator DasR from Streptomyces coelicolor: Implications for the Allosteric Regulation of GntR/HutC Repressors. *PLoS ONE*, **2016**, 11, e0157691	3.7	14
48	Membrane-Mediated Oligomerization of G Protein Coupled Receptors and Its Implications for GPCR Function. *Frontiers in Physiology*, **2016**, 7, 494	4.6	72
47	The Molecular Switching Mechanism at the Conserved D(E)RY Motif in Class-A GPCRs. *Biophysical Journal*, **2016**, 111, 79-89	2.9	9
46	A Critical Comparison of Biomembrane Force Fields: Structure and Dynamics of Model DMPC, POPC, and POPE Bilayers. *Journal of Physical Chemistry B*, **2016**, 120, 3888-903	3.4	95
45	Exploring the Formation and the Structure of Synaptobrevin Oligomers in a Model Membrane. *Biophysical Journal*, **2016**, 110, 2004-15	2.9	11
44	The function of the two-pore channel TPC1 depends on dimerization of its carboxy-terminal helix. *Cellular and Molecular Life Sciences*, **2016**, 73, 2565-81	10.3	20
43	Biomembranes in atomistic and coarse-grained simulations. *Journal of Physics Condensed Matter*, **2015**, 27, 323103	1.8	50
42	Spontaneous adsorption of coiled-coil model peptides K and E to a mixed lipid bilayer. *Journal of Physical Chemistry B*, **2015**, 119, 4396-408	3.4	24
41	Computational Lipidomics with insane: A Versatile Tool for Generating Custom Membranes for Molecular Simulations. *Journal of Chemical Theory and Computation*, **2015**, 11, 2144-55	6.4	504
40	High-Throughput Simulations of Dimer and Trimer Assembly of Membrane Proteins. The DAFT Approach. *Journal of Chemical Theory and Computation*, **2015**, 11, 2278-91	6.4	73

39	Extension of the LOPLS-AA Force Field for Alcohols, Esters, and Monoolein Bilayers and its Validation by Neutron Scattering Experiments. *Journal of Physical Chemistry B*, **2015**, 119, 15287-99	3.4	25
38	Phase Transition of Glycolipid Membranes Studied by Coarse-Grained Simulations. *Langmuir*, **2015**, 31, 9379-87	4	11
37	Synaptobrevin Transmembrane Domain Dimerization Studied by Multiscale Molecular Dynamics Simulations. *Biophysical Journal*, **2015**, 109, 760-71	2.9	17
36	GroPBS: Fast Solver for Implicit Electrostatics of Biomolecules. *Frontiers in Bioengineering and Biotechnology*, **2015**, 3, 186	5.8	2
35	Going Backward: A Flexible Geometric Approach to Reverse Transformation from Coarse Grained to Atomistic Models. *Journal of Chemical Theory and Computation*, **2014**, 10, 676-90	6.4	378
34	Energetic view on membrane pore formation. *Biophysical Journal*, **2014**, 106, 1-2	2.9	11
33	Peptide-induced membrane curvature in edge-stabilized open bilayers: a theoretical and molecular dynamics study. *Journal of Chemical Physics*, **2014**, 141, 024901	3.9	10
32	Going Backward: An Efficient Multiscale Approach using Reverse Transformation. *Biophysical Journal*, **2014**, 106, 640a	2.9	2
31	HLA-B27 and antigen presentation: at the crossroads between immune defense and autoimmunity. *Molecular Immunology*, **2014**, 57, 22-7	4.3	33
30	Molecular dynamics simulations of membrane proteins. *Methods in Molecular Biology*, **2013**, 1033, 85-101	1.4	19
29	Membrane-proximal tryptophans of synaptobrevin II stabilize priming of secretory vesicles. *Journal of Neuroscience*, **2012**, 32, 15983-97	6.6	28
28	Optimization of the OPLS-AA Force Field for Long Hydrocarbons. *Journal of Chemical Theory and Computation*, **2012**, 8, 1459-70	6.4	364
27	Dynamical characterization of two differentially disease associated MHC class I proteins in complex with viral and self-peptides. *Journal of Molecular Biology*, **2012**, 415, 429-42	6.5	60
26	Interaction pattern of Arg 62 in the A-pocket of differentially disease-associated HLA-B27 subtypes suggests distinct TCR binding modes. *PLoS ONE*, **2012**, 7, e32865	3.7	14
25	Mechanism of interaction of monovalent ions with phosphatidylcholine lipid membranes. *Journal of Physical Chemistry B*, **2010**, 114, 9504-9	3.4	81
24	Contribution of charged and polar residues for the formation of the E1-E2 heterodimer from Hepatitis C Virus. *Journal of Molecular Modeling*, **2010**, 16, 1625-37	2	9
23	Predicting free energy changes using structural ensembles. *Nature Methods*, **2009**, 6, 3-4	21.6	196
22	Effects of alkali cations and halide anions on the DOPC lipid membrane. *Journal of Physical Chemistry A*, **2009**, 113, 7235-43	2.8	133

21	Low free energy barrier for ion permeation through double-helical gramicidin. *Journal of Physical Chemistry B*, **2009**, 113, 3195-202	3.4	13
20	Low-affinity peptides and T-cell selection. *Trends in Immunology*, **2009**, 30, 53-60	14.4	29
19	The closure of Pak1-dependent macropinosomes requires the phosphorylation of CtBP1/BARS. *EMBO Journal*, **2008**, 27, 970-81	13	147
18	Kinetics, statistics, and energetics of lipid membrane electroporation studied by molecular dynamics simulations. *Biophysical Journal*, **2008**, 95, 1837-50	2.9	230
17	The influence of 1-alkanols and external pressure on the lateral pressure profiles of lipid bilayers. *Biophysical Journal*, **2008**, 95, 5766-78	2.9	47
16	HLA-B27 subtypes differentially associated with disease exhibit conformational differences in solution. *Journal of Molecular Biology*, **2008**, 376, 798-810	6.5	50
15	Evidence for proton shuffling in a thioredoxin-like protein during catalysis. *Journal of Molecular Biology*, **2008**, 382, 978-86	6.5	9
14	Biomolecular simulations of membranes: physical properties from different force fields. *Journal of Chemical Physics*, **2008**, 128, 125103	3.9	227
13	Molecular determinants of major histocompatibility complex class I complex stability: shaping antigenic features through short and long range electrostatic interactions. *Journal of Biological Chemistry*, **2008**, 283, 23093-103	5.4	17
12	Molecular dynamics simulation of lipids and lipid embossed proteins. *Chemistry and Physics of Lipids* , **2007**, 149, S4	3.7	
11	1-Alkanols and membranes: a story of attraction. *Biochimica Et Biophysica Acta - Biomembranes*, **2007**, 1768, 2899-913	3.8	55
10	Electric field effects on membranes: gramicidin A as a test ground. *Journal of Structural Biology*, **2007**, 157, 545-56	3.4	34
9	High-resolution structures of Escherichia coli cDsbD in different redox states: A combined crystallographic, biochemical and computational study. *Journal of Molecular Biology*, **2006**, 358, 829-45	6.5	34
8	Molekulare Nanomaschinen unter der Lupe: Proteindynamik-Simulationen. *Physik in Unserer Zeit*, **2006**, 37, 73-79	0.1	3
7	Spontaneous formation of detergent micelles around the outer membrane protein OmpX. *Biophysical Journal*, **2005**, 88, 3191-204	2.9	48
6	Differential peptide dynamics is linked to major histocompatibility complex polymorphism. *Journal of Biological Chemistry*, **2004**, 279, 28197-201	5.4	74
5	Multistep binding of divalent cations to phospholipid bilayers: a molecular dynamics study. *Angewandte Chemie - International Edition*, **2004**, 43, 1021-4	16.4	164
4	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	

3	Conformational dynamics of the F1-ATPase beta-subunit: a molecular dynamics study. *Biophysical Journal*, **2003**, 85, 1482-91	2.9	38
2	Effect of sodium chloride on a lipid bilayer. *Biophysical Journal*, **2003**, 85, 1647-55	2.9	452
1	Nanoseconds molecular dynamics simulation of primary mechanical energy transfer steps in F1-ATP synthase. *Nature Structural Biology*, **2002**, 9, 198-202		64