Siewert-Jan Marrink

List of Publications by Year in Descending Order

290 papers	32,667 citations	88 h-index	177 g-index
319 ext. papers	38,101 ext. citations	7.2 avg, IF	7.57 L-index

#	Paper	IF	Citations
290	Polyply; a python suite for facilitating simulations of macromolecules and nanomaterials.. *Nature Communications*, **2022**, 13, 68	17.4	3
289	Membrane thickness, lipid phase and sterol type are determining factors in the permeability of membranes to small solutes.. *Nature Communications*, **2022**, 13, 1605	17.4	4
288	Perspective: a stirring role for metabolism in cells.. *Molecular Systems Biology*, **2022**, 18, e10822	12.2	0
287	Martini 3 Coarse-Grained Force Field: Small Molecules. *Advanced Theory and Simulations*, **2022**, 5, 2100391	3.5	8
286	Complex nanoemulsion for vitamin delivery: droplet organization and interaction with skin membranes.. *Nanoscale*, **2021**,	7.7	1
285	Martini 3 Coarse-Grained Model for Type III Deep Eutectic Solvents: Thermodynamic, Structural, and Extraction Properties. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 17338-17350	8.3	1
284	Bottom-up fabrication of a proteasome-nanopore that unravels and processes single proteins. *Nature Chemistry*, **2021**, 13, 1192-1199	17.6	17
283	Computational Prediction of Transaminase Specificity by a Combination of Docking and Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2021**, 61, 5569-5580	6.1	2
282	Comparing Dimerization Free Energies and Binding Modes of Small Aromatic Molecules with Different Force Fields. *Molecules*, **2021**, 26,	4.8	1
281	Perspectives on High-Throughput Ligand/Protein Docking With Martini MD Simulations. *Frontiers in Molecular Biosciences*, **2021**, 8, 657222	5.6	8
280	Martini 3: a general purpose force field for coarse-grained molecular dynamics. *Nature Methods*, **2021**, 18, 382-388	21.6	124
279	Asymmetric CorA Gating Mechanism as Observed by Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2021**, 61, 2407-2417	6.1	1
278	General Protocol for Constructing Molecular Models of Nanodiscs. *Journal of Chemical Information and Modeling*, **2021**, 61, 2869-2883	6.1	1
277	The Martini Model in Materials Science. *Advanced Materials*, **2021**, 33, e2008635	24	19
276	Capturing Membrane Phase Separation by Dual Resolution Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 5876-5884	6.4	2
275	Semiprocessive Hyperglycosylation of Adhesin by Bacterial Protein -Glycosyltransferases. *ACS Chemical Biology*, **2021**, 16, 165-175	4.9	1
274	Coacervate formation studied by explicit solvent coarse-grain molecular dynamics with the Martini model. *Chemical Science*, **2021**, 12, 8521-8530	9.4	6

273	Biaryl sulfonamides as azosteres for photopharmacology. *Chemical Communications*, **2021**, 57, 4126-4129	6.8	5
272	Fullerene derivatives with oligoethylene-glycol side chains: an investigation on the origin of their outstanding transport properties.. *Journal of Materials Chemistry C*, **2021**, 9, 16217-16225	7.1	1
271	Thermostable D-amino acid decarboxylases derived from Thermotoga maritima diaminopimelate decarboxylase. *Protein Engineering, Design and Selection*, **2021**, 34,	1.9	1
270	A structural view onto disease-linked mutations in the human neutral amino acid exchanger ASCT1. *Computational and Structural Biotechnology Journal*, **2021**, 19, 5246-5254	6.8	0
269	Structure of the human signal peptidase complex reveals the determinants for signal peptide cleavage. *Molecular Cell*, **2021**, 81, 3934-3948.e11	17.6	10
268	Nonconverged Constraints Cause Artificial Temperature Gradients in Lipid Bilayer Simulations. *Journal of Physical Chemistry B*, **2021**, 125, 9537-9546	3.4	4
267	Computational Redesign of an □Transaminase from for Asymmetric Synthesis of Enantiopure Bulky Amines. *ACS Catalysis*, **2021**, 11, 10733-10747	13.1	5
266	Simulating realistic membrane shapes. *Current Opinion in Cell Biology*, **2021**, 71, 103-111	9	9
265	Protocol for Simulations of PEGylated Proteins with Martini 3. *Methods in Molecular Biology*, **2021**, 2199, 315-335	1.4	3
264	Backmapping triangulated surfaces to coarse-grained membrane models. *Nature Communications*, **2020**, 11, 2296	17.4	25
263	Localization Preference of Antimicrobial Peptides on Liquid-Disordered Membrane Domains. *Frontiers in Cell and Developmental Biology*, **2020**, 8, 350	5.7	11
262	Coupling Coarse-Grained to Fine-Grained Models via Hamiltonian Replica Exchange. *Journal of Chemical Theory and Computation*, **2020**, 16, 5313-5322	6.4	5
261	Using Small-Angle Scattering and Contrast Matching to Understand Molecular Packing in Low Molecular Weight Gels. *Matter*, **2020**, 2, 764-778	12.7	24
260	Capturing Choline-Aromatics Cation-□Interactions in the MARTINI Force Field. *Journal of Chemical Theory and Computation*, **2020**, 16, 2550-2560	6.4	15
259	Charge-dependent interactions of monomeric and filamentous actin with lipid bilayers. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 5861-5872	11.5	12
258	Unidirectional rotating molecular motors dynamically interact with adsorbed proteins to direct the fate of mesenchymal stem cells. *Science Advances*, **2020**, 6, eaay2756	14.3	28
257	Membrane mediated toppling mechanism of the folate energy coupling factor transporter. *Nature Communications*, **2020**, 11, 1763	17.4	8
256	Dual Resolution Membrane Simulations Using Virtual Sites. *Journal of Physical Chemistry B*, **2020**, 124, 3944-3953	3.4	8

255	A molecular view on the escape of lipoplexed DNA from the endosome. *ELife*, **2020**, 9,	8.9	15
254	Molecular versus Excitonic Disorder in Individual Artificial Light-Harvesting Systems. *Journal of the American Chemical Society*, **2020**, 142, 18073-18085	16.4	4
253	Piezo1 Forms Specific, Functionally Important Interactions with Phosphoinositides and Cholesterol. *Biophysical Journal*, **2020**, 119, 1683-1697	2.9	24
252	Titratable Martini model for constant pH simulations. *Journal of Chemical Physics*, **2020**, 153, 024118	3.9	20
251	Multiscale modeling of molecular structure and optical properties of complex supramolecular aggregates. *Chemical Science*, **2020**, 11, 11514-11524	9.4	8
250	Asymmetric Synthesis of Optically Pure Aliphatic Amines with an Engineered Robust Transaminase. *Catalysts*, **2020**, 10, 1310	4	3
249	N-type organic thermoelectrics: demonstration of ZT > 0.3. *Nature Communications*, **2020**, 11, 5694	17.4	53
248	Computational and Experimental Advances in Biomembranes: Resolving Their Complexity. *Journal of Physical Chemistry B*, **2020**, 124, 9975-9976	3.4	1
247	Protein-ligand binding with the coarse-grained Martini model. *Nature Communications*, **2020**, 11, 3714	17.4	63
246	Caught in the Act: Mechanistic Insight into Supramolecular Polymerization-Driven Self-Replication from Real-Time Visualization. *Journal of the American Chemical Society*, **2020**, 142, 13709-13717	16.4	17
245	Structural characterization of supramolecular hollow nanotubes with atomistic simulations and SAXS. *Physical Chemistry Chemical Physics*, **2020**, 22, 21083-21093	3.6	4
244	Martini coarse-grained models of imidazolium-based ionic liquids: from nanostructural organization to liquid–liquid extraction. *Green Chemistry*, **2020**, 22, 7376-7386	10	17
243	Resolving Donor–Acceptor Interfaces and Charge Carrier Energy Levels of Organic Semiconductors with Polar Side Chains. *Advanced Functional Materials*, **2020**, 30, 2004799	15.6	14
242	Molecular dynamics simulations in photosynthesis. *Photosynthesis Research*, **2020**, 144, 273-295	3.7	25
241	Molecular mechanism for bidirectional regulation of CD44 for lipid raft affiliation by palmitoylations and PIP2. *PLoS Computational Biology*, **2020**, 16, e1007777	5	6
240	A Practical View of the Martini Force Field. *Methods in Molecular Biology*, **2019**, 2022, 105-127	1.4	21
239	Pitfalls of the Martini Model. *Journal of Chemical Theory and Computation*, **2019**, 15, 5448-5460	6.4	87
238	SWINGER: a clustering algorithm for concurrent coupling of atomistic and supramolecular liquids. *Interface Focus*, **2019**, 9, 20180075	3.9	5

237	Nucleation Mechanisms of Self-Assembled Physisorbed Monolayers on Graphite. *Journal of Physical Chemistry C*, **2019**, 123, 17510-17520	3.8	5
236	Chromophore arrangement in light-harvesting complex II influenced by the protein dynamics on the microsecond time scale. *EPJ Web of Conferences*, **2019**, 205, 09039	0.3	
235	Ceramides bind VDAC2 to trigger mitochondrial apoptosis. *Nature Communications*, **2019**, 10, 1832	17.4	81
234	Lipid Fingerprints and Cofactor Dynamics of Light-Harvesting Complex II in Different Membranes. *Biophysical Journal*, **2019**, 116, 1446-1455	2.9	14
233	Two distinct anionic phospholipid-dependent events involved in SecA-mediated protein translocation. *Biochimica Et Biophysica Acta - Biomembranes*, **2019**, 1861, 183035	3.8	8
232	A Multi-Scale Approach to Membrane Remodeling Processes. *Frontiers in Molecular Biosciences*, **2019**, 6, 59	5.6	7
231	Binding of quinazolinones to c-KIT G-quadruplex; an interplay between hydrogen bonding and □□ stacking. *Biophysical Chemistry*, **2019**, 253, 106220	3.5	6
230	Gangliosides Destabilize Lipid Phase Separation in Multicomponent Membranes. *Biophysical Journal* , **2019**, 117, 1215-1223	2.9	5
229	Serine Phosphorylation of L-Selectin Regulates ERM Binding, Clustering, and Monocyte Protrusion in Transendothelial Migration. *Frontiers in Immunology*, **2019**, 10, 2227	8.4	2
228	Emerging Diversity in Lipid-Protein Interactions. *Chemical Reviews*, **2019**, 119, 5775-5848	68.1	163
227	An Allosteric Pathway in Copper, Zinc Superoxide Dismutase Unravels the Molecular Mechanism of the G93A Amyotrophic Lateral Sclerosis-Linked Mutation. *Journal of Physical Chemistry Letters*, **2019**, 10, 7740-7744	6.4	20
226	Computational Modeling of Realistic Cell Membranes. *Chemical Reviews*, **2019**, 119, 6184-6226	68.1	265
225	Adaption to glucose limitation is modulated by the pleotropic regulator CcpA, independent of selection pressure strength. *BMC Evolutionary Biology*, **2019**, 19, 15	3	10
224	The N-terminal amphipathic helix of Pex11p self-interacts to induce membrane remodelling during peroxisome fission. *Biochimica Et Biophysica Acta - Biomembranes*, **2018**, 1860, 1292-1300	3.8	17
223	Molecular simulations of self-assembling bio-inspired supramolecular systems and their connection to experiments. *Chemical Society Reviews*, **2018**, 47, 3470-3489	58.5	72
222	Multiscale Simulation of Protein Hydration Using the SWINGER Dynamical Clustering Algorithm. *Journal of Chemical Theory and Computation*, **2018**, 14, 1754-1761	6.4	15
221	Structural insights into K48-linked ubiquitin chain formation by the Pex4p-Pex22p complex. *Biochemical and Biophysical Research Communications*, **2018**, 496, 562-567	3.4	4
220	Energetics Underlying Twist Polymorphisms in Amyloid Fibrils. *Journal of Physical Chemistry B*, **2018** , 122, 1081-1091	3.4	31

219	Enhancing Molecular n-Type Doping of Donor-Acceptor Copolymers by Tailoring Side Chains. *Advanced Materials*, **2018**, 30, 1704630	24	157
218	Molecular Dynamics of the Association of L-Selectin and FERM Regulated by PIP2. *Biophysical Journal*, **2018**, 114, 1858-1868	2.9	17
217	Molecular Mechanism of Lipid Nanodisk Formation by Styrene-Maleic Acid Copolymers. *Biophysical Journal*, **2018**, 115, 494-502	2.9	45
216	Fluorinated AlcoholsREffects on Lipid Bilayer Properties. *Biophysical Journal*, **2018**, 115, 679-689	2.9	15
215	Lipid-Protein Interactions Are Unique Fingerprints for Membrane Proteins. *ACS Central Science*, **2018**, 4, 709-717	16.8	139
214	Curvature-Induced Sorting of Lipids in Plasma Membrane Tethers. *Advanced Theory and Simulations*, **2018**, 1, 1800034	3.5	28
213	Role of Charge and Hydrophobicity in Liprotide Formation: A Molecular Dynamics Study with Experimental Constraints. *ChemBioChem*, **2018**, 19, 263-271	3.8	7
212	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. *Journal of Membrane Biology*, **2018**, 251, 609-631	2.3	26
211	Cholesterol Flip-Flop Impacts Domain Registration in Plasma Membrane Models. *Journal of Physical Chemistry Letters*, **2018**, 9, 5527-5533	6.4	28
210	Transferable MARTINI Model of Poly(ethylene Oxide). *Journal of Physical Chemistry B*, **2018**, 122, 7436-7449	3.4	62
209	High-Throughput Simulations Reveal Membrane-Mediated Effects of Alcohols on MscL Gating. *Journal of the American Chemical Society*, **2017**, 139, 2664-2671	16.4	24
208	Bulk Heterojunction Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations. *Journal of the American Chemical Society*, **2017**, 139, 3697-3705	16.4	99
207	Design and Properties of Genetically Encoded Probes for Sensing Macromolecular Crowding. *Biophysical Journal*, **2017**, 112, 1929-1939	2.9	36
206	Exchange pathways of plastoquinone and plastoquinol in the photosystem II complex. *Nature Communications*, **2017**, 8, 15214	17.4	46
205	Martini Coarse-Grained Force Field: Extension to RNA. *Biophysical Journal*, **2017**, 113, 246-256	2.9	74
204	Insight into the complete substrate-binding pocket of ThiT by chemical and genetic mutations. *MedChemComm*, **2017**, 8, 1121-1130	5	11
203	Lipid-Protein Interactions are Unique Fingerprints for Membrane Proteins. *Biophysical Journal*, **2017** , 112, 84a	2.9	2
202	Stability and dynamics of membrane-spanning DNA nanopores. *Nature Communications*, **2017**, 8, 14784	17.4	36

201	Lipid and Peptide Diffusion in Bilayers: The Saffman-Delbrück Model and Periodic Boundary Conditions. *Journal of Physical Chemistry B*, **2017**, 121, 3443-3457	3.4	69
200	Enhancing doping efficiency by improving host-dopant miscibility for fullerene-based n-type thermoelectrics. *Journal of Materials Chemistry A*, **2017**, 5, 21234-21241	13	56
199	Structural and Spectroscopic Properties of Assemblies of Self-Replicating Peptide Macrocycles. *ACS Nano*, **2017**, 11, 7858-7868	16.7	30
198	cgHeliParm: analysis of dsDNA helical parameters for coarse-grained MARTINI molecular dynamics simulations. *Bioinformatics*, **2017**, 33, 3813-3815	7.2	1
197	Computational Lipidomics of the Neuronal Plasma Membrane. *Biophysical Journal*, **2017**, 113, 2271-2280	2.9	112
196	Ganglioside-Lipid and Ganglioside-Protein Interactions Revealed by Coarse-Grained and Atomistic Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 3262-3275	3.4	60
195	Molecular Dynamics of Photosystem II Embedded in the Thylakoid Membrane. *Journal of Physical Chemistry B*, **2017**, 121, 3237-3249	3.4	23
194	Prediction of Thylakoid Lipid Binding Sites on Photosystem II. *Biophysical Journal*, **2017**, 113, 2669-2681	2.9	21
193	Alcohol Interactions with Lipid Bilayers. *Molecules*, **2017**, 22,	4.8	21
192	Lipid phase separation in the presence of hydrocarbons in giant unilamellar vesicles. *AIMS Biophysics*, **2017**, 4, 528-542	0.8	3
191	Martini straight: Boosting performance using a shorter cutoff and GPUs. *Computer Physics Communications*, **2016**, 199, 1-7	4.2	221
190	Adaptive Resolution Simulation of Supramolecular Water: The Concurrent Making, Breaking, and Remaking of Water Bundles. *Journal of Chemical Theory and Computation*, **2016**, 12, 4138-45	6.4	26
189	Adaptive resolution simulation of an atomistic DNA molecule in MARTINI salt solution. *European Physical Journal: Special Topics*, **2016**, 225, 1595-1607	2.3	22
188	Coupled binding mechanism of three sodium ions and aspartate in the glutamate transporter homologue Glt. *Nature Communications*, **2016**, 7, 13420	17.4	69
187	Altered secondary structure of Dynorphin A associates with loss of opioid signalling and NMDA-mediated excitotoxicity in SCA23. *Human Molecular Genetics*, **2016**, 25, 2728-2737	5.6	7
186	Molecular mechanism of cardiolipin-mediated assembly of respiratory chain supercomplexes. *Chemical Science*, **2016**, 7, 4435-4443	9.4	57
185	Computational RmicroscopyRof cellular membranes. *Journal of Cell Science*, **2016**, 129, 257-68	5.3	96
184	An Amphotericin B Derivative Equally Potent to Amphotericin B and with Increased Safety. *PLoS ONE*, **2016**, 11, e0162171	3.7	15

183	Ironing out their differences: dissecting the structural determinants of a phenylalanine aminomutase and ammonia lyase. *ACS Chemical Biology*, **2015**, 10, 989-97	4.9	21
182	Lipid Organization of the Plasma Membrane. *Biophysical Journal*, **2015**, 108, 358a	2.9	3
181	Martini Coarse-Grained Force Field: Extension to DNA. *Journal of Chemical Theory and Computation*, **2015**, 11, 3932-45	6.4	156
180	Atomistic and Coarse Grain Topologies for the Cofactors Associated with the Photosystem II Core Complex. *Journal of Physical Chemistry B*, **2015**, 119, 7791-803	3.4	27
179	Characterization of thylakoid lipid membranes from cyanobacteria and higher plants by molecular dynamics simulations. *Biochimica Et Biophysica Acta - Biomembranes*, **2015**, 1848, 1319-30	3.8	94
178	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
177	Benchmark of Schemes for Multiscale Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2015**, 11, 1389-98	6.4	21
176	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
175	Adaptive resolution simulation of polarizable supramolecular coarse-grained water models. *Journal of Chemical Physics*, **2015**, 142, 244118	3.9	39
174	CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field. *Journal of Chemical Theory and Computation*, **2015**, 11, 4486-94	6.4	181
173	Hsc70-4 Deforms Membranes to Promote Synaptic Protein Turnover by Endosomal Microautophagy. *Neuron*, **2015**, 88, 735-48	13.9	111
172	Intramolecular photostabilization via triplet-state quenching: design principles to make organic fluorophores "self-healing". *Faraday Discussions*, **2015**, 184, 221-35	3.6	22
171	Dry Martini, a coarse-grained force field for lipid membrane simulations with implicit solvent. *Journal of Chemical Theory and Computation*, **2015**, 11, 260-75	6.4	181
170	From light-harvesting to photoprotection: structural basis of the dynamic switch of the major antenna complex of plants (LHCII). *Scientific Reports*, **2015**, 5, 15661	4.9	79
169	Parameters for Martini sterols and hopanoids based on a virtual-site description. *Journal of Chemical Physics*, **2015**, 143, 243152	3.9	82
168	Enantioselective enzymes by computational design and in silico screening. *Angewandte Chemie - International Edition*, **2015**, 54, 3726-30	16.4	88
167	MARTINI coarse-grained model for crystalline cellulose microfibers. *Journal of Physical Chemistry B*, **2015**, 119, 465-73	3.4	39
166	Enantioselective Enzymes by Computational Design and In Silico Screening. *Angewandte Chemie*, **2015**, 127, 3797-3801	3.6	17

165	Helfrich model of membrane bending: from Gibbs theory of liquid interfaces to membranes as thick anisotropic elastic layers. *Advances in Colloid and Interface Science*, **2014**, 208, 25-33	14.3	53
164	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
163	Establishing conditions for simulating hydrophobic solutes in electric fields by molecular dynamics: effects of the long-range van der Waals treatment on the apparent particle mobility. *Journal of Molecular Modeling*, **2014**, 20, 2359	2	2
162	Computational library design for increasing haloalkane dehalogenase stability. *ChemBioChem*, **2014** , 15, 1660-72	3.8	52
161	Global structural changes of an ion channel during its gating are followed by ion mobility mass spectrometry. *Proceedings of the National Academy of Sciences of the United States of America*, **2014** , 111, 17170-5	11.5	54
160	Lipid organization of the plasma membrane. *Journal of the American Chemical Society*, **2014**, 136, 14554-9	26.4	519
159	Phytochemicals perturb membranes and promiscuously alter protein function. *ACS Chemical Biology*, **2014**, 9, 1788-98	4.9	184
158	Disaccharides impact the lateral organization of lipid membranes. *Journal of the American Chemical Society*, **2014**, 136, 16167-75	16.4	40
157	Computationally efficient and accurate enantioselectivity modeling by clusters of molecular dynamics simulations. *Journal of Chemical Information and Modeling*, **2014**, 54, 2079-92	6.1	33
156	The activation mode of the mechanosensitive ion channel, MscL, by lysophosphatidylcholine differs from tension-induced gating. *FASEB Journal*, **2014**, 28, 4292-302	0.9	36
155	Adaptive Resolution Simulation of MARTINI Solvents. *Journal of Chemical Theory and Computation*, **2014**, 10, 2591-8	6.4	39
154	Hydrophobic compounds reshape membrane domains. *PLoS Computational Biology*, **2014**, 10, e1003873	5	42
153	Simulation of polyethylene glycol and calcium-mediated membrane fusion. *Journal of Chemical Physics*, **2014**, 140, 124905	3.9	36
152	Adaptive resolution simulation of an atomistic protein in MARTINI water. *Journal of Chemical Physics*, **2014**, 140, 054114	3.9	66
151	Computationally designed libraries for rapid enzyme stabilization. *Protein Engineering, Design and Selection*, **2014**, 27, 49-58	1.9	164
150	Mechanisms shaping cell membranes. *Current Opinion in Cell Biology*, **2014**, 29, 53-60	9	154
149	The power of coarse graining in biomolecular simulations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 225-248	7.9	346
148	Perspective on the Martini model. *Chemical Society Reviews*, **2013**, 42, 6801-22	58.5	805

147	Defined lipid analogues induce transient channels to facilitate drug-membrane traversal and circumvent cancer therapy resistance. *Scientific Reports*, **2013**, 3, 1949	4.9	18
146	Interbilayer repulsion forces between tension-free lipid bilayers from simulation. *Soft Matter*, **2013**, 9, 10705	3.6	16
145	Coarse-grain modelling of protein-protein interactions. *Current Opinion in Structural Biology*, **2013**, 23, 878-86	8.1	108
144	Identification of cardiolipin binding sites on cytochrome c oxidase at the entrance of proton channels. *Scientific Reports*, **2013**, 3, 1263	4.9	112
143	The Martini coarse-grained force field. *Methods in Molecular Biology*, **2013**, 924, 533-65	1.4	79
142	Improved Parameters for the Martini Coarse-Grained Protein Force Field. *Journal of Chemical Theory and Computation*, **2013**, 9, 687-97	6.4	782
141	Mixing MARTINI: electrostatic coupling in hybrid atomistic-coarse-grained biomolecular simulations. *Journal of Physical Chemistry B*, **2013**, 117, 3516-30	3.4	117
140	Martini Force Field Parameters for Glycolipids. *Journal of Chemical Theory and Computation*, **2013**, 9, 1694-708	6.4	127
139	Semiconducting single-walled carbon nanotubes on demand by polymer wrapping. *Advanced Materials*, **2013**, 25, 2948-56	24	152
138	Improved Angle Potentials for Coarse-Grained Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2013**, 9, 3282-92	6.4	45
137	Vibrational Spectra of a Mechanosensitive Channel. *Journal of Physical Chemistry Letters*, **2013**, 4, 448-52	6.4	22
136	Computational microscopy of cyclodextrin mediated cholesterol extraction from lipid model membranes. *Scientific Reports*, **2013**, 3, 2071	4.9	84
135	MARTINI Model for Physisorption of Organic Molecules on Graphite. *Journal of Physical Chemistry C* , **2013**, 117, 15623-15631	3.8	30
134	Evidence for cardiolipin binding sites on the membrane-exposed surface of the cytochrome bc1. *Journal of the American Chemical Society*, **2013**, 135, 3112-20	16.4	126
133	Molecular view on protein sorting into liquid-ordered membrane domains mediated by gangliosides and lipid anchors. *Faraday Discussions*, **2013**, 161, 347-63; discussion 419-59	3.6	63
132	Gaussian curvature elasticity determined from global shape transformations and local stress distributions: a comparative study using the MARTINI model. *Faraday Discussions*, **2013**, 161, 365-82; discussion 419-59	3.6	68
131	Anomalous viscosity effect in the early stages of the ion-assisted adhesion/fusion event between lipid bilayers: a theoretical and computational study. *Journal of Chemical Physics*, **2013**, 138, 234901	3.9	3
130	Dual action of BPC194: a membrane active peptide killing bacterial cells. *PLoS ONE*, **2013**, 8, e61541	3.7	13

129	Molecular plasticity regulates oligomerization and cytotoxicity of the multipeptide-length amyloid-peptide pool. *Journal of Biological Chemistry*, **2012**, 287, 36732-43	5.4	29
128	Rhodopsin forms a dimer with cytoplasmic helix 8 contacts in native membranes. *Biochemistry*, **2012**, 51, 1819-21	3.2	57
127	Efficient Algorithms for Langevin and DPD Dynamics. *Journal of Chemical Theory and Computation*, **2012**, 8, 3637-49	6.4	157
126	Transmembrane helices can induce domain formation in crowded model membranes. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 984-94	3.8	102
125	Dimerization of Amino Acid Side Chains: Lessons from the Comparison of Different Force Fields. *Journal of Chemical Theory and Computation*, **2012**, 8, 1003-14	6.4	49
124	Amylose folding under the influence of lipids. *Carbohydrate Research*, **2012**, 364, 1-7	2.9	52
123	Structural determinants of the supramolecular organization of G protein-coupled receptors in bilayers. *Journal of the American Chemical Society*, **2012**, 134, 10959-65	16.4	181
122	In silico design of robust bolalipid membranes. *Biomacromolecules*, **2012**, 13, 196-205	6.9	34
121	Molecular view of the role of fusion peptides in promoting positive membrane curvature. *Journal of the American Chemical Society*, **2012**, 134, 1543-52	16.4	67
120	Molecular structure of membrane tethers. *Biophysical Journal*, **2012**, 102, 1866-71	2.9	54
119	Structural investigation of MscL gating using experimental data and coarse grained MD simulations. *PLoS Computational Biology*, **2012**, 8, e1002683	5	37
118	GPU-SD and DPD parallelization for Gromacs tools for molecular dynamics simulations **2012**,		3
117	Line-tension controlled mechanism for influenza fusion. *PLoS ONE*, **2012**, 7, e38302	3.7	51
116	Protein shape change has a major effect on the gating energy of a mechanosensitive channel. *Biophysical Journal*, **2011**, 100, 1651-9	2.9	45
115	The molecular basis for antimicrobial activity of pore-forming cyclic peptides. *Biophysical Journal*, **2011**, 100, 2422-31	2.9	58
114	Curvature-dependent elastic properties of liquid-ordered domains result in inverted domain sorting on uniaxially compressed vesicles. *Physical Review Letters*, **2011**, 106, 148102	7.4	36
113	Hybrid simulations: combining atomistic and coarse-grained force fields using virtual sites. *Physical Chemistry Chemical Physics*, **2011**, 13, 10437-48	3.6	153
112	Low density lipoprotein: structure, dynamics, and interactions of apoB-100 with lipids. *Soft Matter*, **2011**, 7, 8135	3.6	38

111	The effect of aliphatic alcohols on fluid bilayers in unilamellar DOPC vesicles--a small-angle neutron scattering and molecular dynamics study. *Biochimica Et Biophysica Acta - Biomembranes*, **2011**, 1808, 2136-46	3.8	24
110	Structural basis for the enhanced activity of cyclic antimicrobial peptides: the case of BPC194. *Biochimica Et Biophysica Acta - Biomembranes*, **2011**, 1808, 2197-205	3.8	43
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