Siewert-Jan Marrink

List of Publications by Year
in descending order

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292 papers	42,619 citations	2696 98 h-index	3037 194 g-index
319 all docs	319 docs citations	319 times ranked	26221 citing authors

#	Article	IF	Citations
1	Two decades of Martini: Better beads, broader scope. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	58
2	Polyply; a python suite for facilitating simulations of macromolecules and nanomaterials. Nature Communications, 2022, 13, 68.	5.8	48
3	Complex nanoemulsion for vitamin delivery: droplet organization and interaction with skin membranes. Nanoscale, 2022, 14, 506-514.	2.8	19
4	Protein dynamics and lipid affinity of monomeric, zeaxanthin-binding LHCII in thylakoid membranes. Biophysical Journal, 2022, 121, 396-409.	0.2	9
5	Membrane thickness, lipid phase and sterol type are determining factors in the permeability of membranes to small solutes. Nature Communications, 2022, 13, 1605.	5.8	81
6	Perspective: a stirring role for metabolism in cells. Molecular Systems Biology, 2022, 18, e10822.	3.2	12
7	Martini 3 Coarseâ€Grained Force Field: Small Molecules. Advanced Theory and Simulations, 2022, 5, .	1.3	72
8	Modelling structural properties of cyanine dye nanotubes at coarse-grained level. Nanoscale Advances, 2022, 4, 3033-3042.	2.2	5
9	Quantification of Protein Glycosylation Using Nanopores. Nano Letters, 2022, 22, 5357-5364.	4.5	29
10	Semiprocessive Hyperglycosylation of Adhesin by Bacterial Protein N-Glycosyltransferases. ACS Chemical Biology, 2021, 16, 165-175.	1.6	6
11	Coacervate formation studied by explicit solvent coarse-grain molecular dynamics with the Martini model. Chemical Science, 2021, 12, 8521-8530.	3.7	37
12	Biaryl sulfonamides as cisoid azosteres for photopharmacology. Chemical Communications, 2021, 57, 4126-4129.	2.2	9
13	Fullerene derivatives with oligoethyleneâ€“glycol side chains: an investigation on the origin of their outstanding transport properties. Journal of Materials Chemistry C, 2021, 9, 16217-16225.	2.7	10
14	Thermostable D-amino acid decarboxylases derived from Thermotoga maritima diaminopimelate decarboxylase. Protein Engineering, Design and Selection, 2021, 34, .	1.0	2
15	A structural view onto disease-linked mutations in the human neutral amino acid exchanger ASCT1. Computational and Structural Biotechnology Journal, 2021, 19, 5246-5254.	1.9	9
16	Perspectives on High-Throughput Ligand/Protein Docking With Martini MD Simulations. Frontiers in Molecular Biosciences, 2021, 8, 657222.	1.6	25
17	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	9.0	557
18	Asymmetric CorA Gating Mechanism as Observed by Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2021, 61, 2407-2417.	2.5	10

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19	General Protocol for Constructing Molecular Models of Nanodiscs. Journal of Chemical Information and Modeling, 2021, 61, 2869-2883.	2.5	11
20	The Martini Model in Materials Science. Advanced Materials, 2021, 33, e2008635.	11.1	63
21	Capturing Membrane Phase Separation by Dual Resolution Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2021, 17, 5876-5884.	2.3	10
22	Structure of the human signal peptidase complex reveals the determinants for signal peptide cleavage. Molecular Cell, 2021, 81, 3934-3948.e11.	4.5	51
23	Nonconverged Constraints Cause Artificial Temperature Gradients in Lipid Bilayer Simulations. Journal of Physical Chemistry B, 2021, 125, 9537-9546.	1.2	28
24	Computational Redesign of an Ï‰-Transaminase from Pseudomonas jessenii for Asymmetric Synthesis of Enantiopure Bulky Amines. ACS Catalysis, 2021, 11, 10733-10747.	5.5	28
25	Simulating realistic membrane shapes. Current Opinion in Cell Biology, 2021, 71, 103-111.	2.6	45
26	Protocol for Simulations of PEGylated Proteins with Martini 3. Methods in Molecular Biology, 2021, 2199, 315-335.	0.4	10
27	Computational Prediction of Ï‰-Transaminase Specificity by a Combination of Docking and Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2021, 61, 5569-5580.	2.5	17
28	Sequential Voxel-Based Leaflet Segmentation of Complex Lipid Morphologies. Journal of Chemical Theory and Computation, 2021, 17, 7873-7885.	2.3	8
29	Comparing Dimerization Free Energies and Binding Modes of Small Aromatic Molecules with Different Force Fields. Molecules, 2021, 26, 6069.	1.7	3
30	Bottom-up fabrication of a proteasomeâ€“nanopore that unravels and processes single proteins. Nature Chemistry, 2021, 13, 1192-1199.	6.6	76
31	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.	3.2	20
32	Molecular versus Excitonic Disorder in Individual Artificial Light-Harvesting Systems. Journal of the American Chemical Society, 2020, 142, 18073-18085.	6.6	13
33	Piezo1 Forms Specific, Functionally Important Interactions with Phosphoinositides and Cholesterol. Biophysical Journal, 2020, 119, 1683-1697.	0.2	60
34	Titratable Martini model for constant pH simulations. Journal of Chemical Physics, 2020, 153, 024118.	1.2	57
35	Multiscale modeling of molecular structure and optical properties of complex supramolecular aggregates. Chemical Science, 2020, 11, 11514-11524.	3.7	18
36	Asymmetric Synthesis of Optically Pure Aliphatic Amines with an Engineered Robust Ï‰-Transaminase. Catalysts, 2020, 10, 1310.	1.6	10

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37	N-type organic thermoelectrics: demonstration of ZTâ€‰>â€‰0.3. Nature Communications, 2020, 11, 5694.	5.8	98
38	Computational and Experimental Advances in Biomembranes: Resolving Their Complexity. Journal of Physical Chemistry B, 2020, 124, 9975-9976.	1.2	3
39	Proteinâ€“ligand binding with the coarse-grained Martini model. Nature Communications, 2020, 11, 3714.	5.8	139
40	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.	6.6	44
41	Structural characterization of supramolecular hollow nanotubes with atomistic simulations and SAXS. Physical Chemistry Chemical Physics, 2020, 22, 21083-21093.	1.3	14
42	Martini coarse-grained models of imidazolium-based ionic liquids: from nanostructural organization to liquidâ€“liquid extraction. Green Chemistry, 2020, 22, 7376-7386.	4.6	45
43	Resolving Donorâ€“Acceptor Interfaces and Charge Carrier Energy Levels of Organic Semiconductors with Polar Side Chains. Advanced Functional Materials, 2020, 30, 2004799.	7.8	28
44	Backmapping triangulated surfaces to coarse-grained membrane models. Nature Communications, 2020, 11, 2296.	5.8	86
45	Localization Preference of Antimicrobial Peptides on Liquid-Disordered Membrane Domains. Frontiers in Cell and Developmental Biology, 2020, 8, 350.	1.8	25
46	Coupling Coarse-Grained to Fine-Grained Models via Hamiltonian Replica Exchange. Journal of Chemical Theory and Computation, 2020, 16, 5313-5322.	2.3	9
47	Using Small-Angle Scattering and Contrast Matching to Understand Molecular Packing in Low Molecular Weight Gels. Matter, 2020, 2, 764-778.	5.0	49
48	Capturing Cholineâ€“Aromatics Cationâˆ’Ï€ Interactions in the MARTINI Force Field. Journal of Chemical Theory and Computation, 2020, 16, 2550-2560.	2.3	35
49	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.	3.3	35
50	Unidirectional rotating molecular motors dynamically interact with adsorbed proteins to direct the fate of mesenchymal stem cells. Science Advances, 2020, 6, eaay2756.	4.7	42
51	Membrane mediated toppling mechanism of the folate energy coupling factor transporter. Nature Communications, 2020, 11, 1763.	5.8	21
52	Dual Resolution Membrane Simulations Using Virtual Sites. Journal of Physical Chemistry B, 2020, 124, 3944-3953.	1.2	21
53	Molecular dynamics simulations in photosynthesis. Photosynthesis Research, 2020, 144, 273-295.	1.6	50
54	Molecular mechanism for bidirectional regulation of CD44 for lipid raft affiliation by palmitoylations and PIP2. PLoS Computational Biology, 2020, 16, e1007777.	1.5	22

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55	A molecular view on the escape of lipoplexed DNA from the endosome. ELife, 2020, 9, .	2.8	46
56	Two distinct anionic phospholipid-dependent events involved in SecA-mediated protein translocation. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 183035.	1.4	16
57	A Multi-Scale Approach to Membrane Remodeling Processes. Frontiers in Molecular Biosciences, 2019, 6, 59.	1.6	19
58	Binding of quinazolinones to c-KIT G-quadruplex; an interplay between hydrogen bonding and Ï€-Ï€ stacking. Biophysical Chemistry, 2019, 253, 106220.	1.5	11
59	Gangliosides Destabilize Lipid Phase Separation in Multicomponent Membranes. Biophysical Journal, 2019, 117, 1215-1223.	0.2	9
60	Serine Phosphorylation of L-Selectin Regulates ERM Binding, Clustering, and Monocyte Protrusion in Transendothelial Migration. Frontiers in Immunology, 2019, 10, 2227.	2.2	6
61	A Practical View of the Martini Force Field. Methods in Molecular Biology, 2019, 2022, 105-127.	0.4	38
62	Pitfalls of the Martini Model. Journal of Chemical Theory and Computation, 2019, 15, 5448-5460.	2.3	159
63	SWINGER: a clustering algorithm for concurrent coupling of atomistic and supramolecular liquids. Interface Focus, 2019, 9, 20180075.	1.5	11
64	Nucleation Mechanisms of Self-Assembled Physisorbed Monolayers on Graphite. Journal of Physical Chemistry C, 2019, 123, 17510-17520.	1.5	15
65	Chromophore arrangement in light-harvesting complex II influenced by the protein dynamics on the microsecond time scale. EPJ Web of Conferences, 2019, 205, 09039.	0.1	0
66	Ceramides bind VDAC2 to trigger mitochondrial apoptosis. Nature Communications, 2019, 10, 1832.	5.8	144
67	Lipid Fingerprints and Cofactor Dynamics of Light-Harvesting Complex II in Different Membranes. Biophysical Journal, 2019, 116, 1446-1455.	0.2	31
68	Emerging Diversity in Lipidâ€“Protein Interactions. Chemical Reviews, 2019, 119, 5775-5848.	23.0	299
69	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.	2.1	49
70	Computational Modeling of Realistic Cell Membranes. Chemical Reviews, 2019, 119, 6184-6226.	23.0	502
71	Adaption to glucose limitation is modulated by the pleotropic regulator CcpA, independent of selection pressure strength. BMC Evolutionary Biology, 2019, 19, 15.	3.2	19
72	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.	1.4	28

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73	Molecular simulations of self-assembling bio-inspired supramolecular systems and their connection to experiments. Chemical Society Reviews, 2018, 47, 3470-3489.	18.7	119
74	Multiscale Simulation of Protein Hydration Using the SWINGER Dynamical Clustering Algorithm. Journal of Chemical Theory and Computation, 2018, 14, 1754-1761.	2.3	19
75	Structural insights into K48-linked ubiquitin chain formation by the Pex4p-Pex22p complex. Biochemical and Biophysical Research Communications, 2018, 496, 562-567.	1.0	6
76	Energetics Underlying Twist Polymorphisms in Amyloid Fibrils. Journal of Physical Chemistry B, 2018, 122, 1081-1091.	1.2	44
77	Enhancing Molecular nâ€Type Doping of Donorâ€“Acceptor Copolymers by Tailoring Side Chains. Advanced Materials, 2018, 30, 1704630.	11.1	217
78	Molecular Dynamics of the Association of L-Selectin and FERM Regulated by PIP2. Biophysical Journal, 2018, 114, 1858-1868.	0.2	33
79	Role of Charge and Hydrophobicity in Liprotide Formation: A Molecular Dynamics Study with Experimental Constraints. ChemBioChem, 2018, 19, 263-271.	1.3	11
80	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. Journal of Membrane Biology, 2018, 251, 609-631.	1.0	33
81	Cholesterol Flip-Flop Impacts Domain Registration in Plasma Membrane Models. Journal of Physical Chemistry Letters, 2018, 9, 5527-5533.	2.1	36
82	Transferable MARTINI Model of Poly(ethylene Oxide). Journal of Physical Chemistry B, 2018, 122, 7436-7449.	1.2	99
83	Molecular Mechanism of Lipid Nanodisk Formation by Styrene-Maleic Acid Copolymers. Biophysical Journal, 2018, 115, 494-502.	0.2	64
84	Fluorinated Alcoholsâ€™ Effects on Lipid Bilayer Properties. Biophysical Journal, 2018, 115, 679-689.	0.2	23
85	Lipidâ€“Protein Interactions Are Unique Fingerprints for Membrane Proteins. ACS Central Science, 2018, 4, 709-717.	5.3	274
86	Curvatureâ€Induced Sorting of Lipids in Plasma Membrane Tethers. Advanced Theory and Simulations, 2018, 1, 1800034.	1.3	54
87	High-Throughput Simulations Reveal Membrane-Mediated Effects of Alcohols on MscL Gating. Journal of the American Chemical Society, 2017, 139, 2664-2671.	6.6	41
88	Bulk Heterojunction Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations. Journal of the American Chemical Society, 2017, 139, 3697-3705.	6.6	133
89	Design and Properties of Genetically Encoded Probes for Sensing Macromolecular Crowding. Biophysical Journal, 2017, 112, 1929-1939.	0.2	61
90	Exchange pathways of plastoquinone and plastoquinol in the photosystem II complex. Nature Communications, 2017, 8, 15214.	5.8	71

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91	Martini Coarse-Grained Force Field: Extension to RNA. Biophysical Journal, 2017, 113, 246-256.	0.2	156
92	Insight into the complete substrate-binding pocket of ThiT by chemical and genetic mutations. MedChemComm, 2017, 8, 1121-1130.	3.5	16
93	Lipid-Protein Interactions are Unique Fingerprints for Membrane Proteins. Biophysical Journal, 2017, 112, 84a.	0.2	2
94	Stability and dynamics of membrane-spanning DNA nanopores. Nature Communications, 2017, 8, 14784.	5.8	61
95	Lipid and Peptide Diffusion in Bilayers: The Saffmanâ€“DelbrÃ¼ck Model and Periodic Boundary Conditions. Journal of Physical Chemistry B, 2017, 121, 3443-3457.	1.2	91
96	Enhancing doping efficiency by improving host-dopant miscibility for fullerene-based n-type thermoelectrics. Journal of Materials Chemistry A, 2017, 5, 21234-21241.	5.2	73
97	Structural and Spectroscopic Properties of Assemblies of Self-Replicating Peptide Macrocycles. ACS Nano, 2017, 11, 7858-7868.	7.3	36
98	cgHeliParm: analysis of dsDNA helical parameters for coarse-grained MARTINI molecular dynamics simulations. Bioinformatics, 2017, 33, 3813-3815.	1.8	3
99	CHARMMâ€GUI Martini Maker for modeling and simulation of complex bacterial membranes with lipopolysaccharides. Journal of Computational Chemistry, 2017, 38, 2354-2363.	1.5	150
100	Computational Lipidomics of the Neuronal Plasma Membrane. Biophysical Journal, 2017, 113, 2271-2280.	0.2	197
101	Ganglioside-Lipid and Ganglioside-Protein Interactions Revealed by Coarse-Grained and Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 3262-3275.	1.2	81
102	Molecular Dynamics of Photosystem II Embedded in the Thylakoid Membrane. Journal of Physical Chemistry B, 2017, 121, 3237-3249.	1.2	34
103	Prediction of Thylakoid Lipid Binding Sites on Photosystem II. Biophysical Journal, 2017, 113, 2669-2681.	0.2	37
104	Alcohol Interactions with Lipid Bilayers. Molecules, 2017, 22, 2078.	1.7	28
105	Lipid phase separation in the presence of hydrocarbons in giant unilamellar vesicles. AIMS Biophysics, 2017, 4, 528-542.	0.3	5
106	An Amphotericin B Derivative Equally Potent to Amphotericin B and with Increased Safety. PLoS ONE, 2016, 11, e0162171.	1.1	29
107	Adaptive Resolution Simulation of Supramolecular Water: The Concurrent Making, Breaking, and Remaking of Water Bundles. Journal of Chemical Theory and Computation, 2016, 12, 4138-4145.	2.3	30
108	Adaptive resolution simulation of an atomistic DNA molecule in MARTINI salt solution. European Physical Journal: Special Topics, 2016, 225, 1595-1607.	1.2	25

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109	Coupled binding mechanism of three sodium ions and aspartate in the glutamate transporter homologue GltTk. Nature Communications, 2016, 7, 13420.	5.8	93
110	Altered secondary structure of Dynorphin A associates with loss of opioid signalling and NMDA-mediated excitotoxicity in SCA23. Human Molecular Genetics, 2016, 25, ddw130.	1.4	9
111	Molecular mechanism of cardiolipin-mediated assembly of respiratory chain supercomplexes. Chemical Science, 2016, 7, 4435-4443.	3.7	80
112	Computational â€˜microscopyâ€™ of cellular membranes. Journal of Cell Science, 2016, 129, 257-68.	1.2	119
113	Martini straight: Boosting performance using a shorter cutoff and GPUs. Computer Physics Communications, 2016, 199, 1-7.	3.0	352
114	From light-harvesting to photoprotection: structural basis of the dynamic switch of the major antenna complex of plants (LHCII). Scientific Reports, 2015, 5, 15661.	1.6	108
115	Parameters for Martini sterols and hopanoids based on a virtual-site description. Journal of Chemical Physics, 2015, 143, 243152.	1.2	125
116	Enantioselective Enzymes by Computational Design and In Silico Screening. Angewandte Chemie - International Edition, 2015, 54, 3726-3730.	7.2	119
117	MARTINI Coarse-Grained Model for Crystalline Cellulose Microfibers. Journal of Physical Chemistry B, 2015, 119, 465-473.	1.2	54
118	Ironing out Their Differences: Dissecting the Structural Determinants of a Phenylalanine Aminomutase and Ammonia Lyase. ACS Chemical Biology, 2015, 10, 989-997.	1.6	23
119	Lipid Organization of the Plasma Membrane. Biophysical Journal, 2015, 108, 358a.	0.2	7
120	Martini Coarse-Grained Force Field: Extension to DNA. Journal of Chemical Theory and Computation, 2015, 11, 3932-3945.	2.3	239
121	Atomistic and Coarse Grain Topologies for the Cofactors Associated with the Photosystem II Core Complex. Journal of Physical Chemistry B, 2015, 119, 7791-7803.	1.2	41
122	Characterization of thylakoid lipid membranes from cyanobacteria and higher plants by molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 1319-1330.	1.4	120
123	Computational Lipidomics with insane: A Versatile Tool for Generating Custom Membranes for Molecular Simulations. Journal of Chemical Theory and Computation, 2015, 11, 2144-2155.	2.3	847
124	Benchmark of Schemes for Multiscale Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2015, 11, 1389-1398.	2.3	24
125	High-Throughput Simulations of Dimer and Trimer Assembly of Membrane Proteins. The DAFT Approach. Journal of Chemical Theory and Computation, 2015, 11, 2278-2291.	2.3	94
126	Adaptive resolution simulation of polarizable supramolecular coarse-grained water models. Journal of Chemical Physics, 2015, 142, 244118.	1.2	39

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127	CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field. Journal of Chemical Theory and Computation, 2015, 11, 4486-4494.	2.3	340
128	Hsc70-4 Deforms Membranes to Promote Synaptic Protein Turnover by Endosomal Microautophagy. Neuron, 2015, 88, 735-748.	3.8	140
129	Intramolecular photostabilization via triplet-state quenching: design principles to make organic fluorophores â€œself-healingâ€. Faraday Discussions, 2015, 184, 221-235.	1.6	31
130	Dry Martini, a Coarse-Grained Force Field for Lipid Membrane Simulations with Implicit Solvent. Journal of Chemical Theory and Computation, 2015, 11, 260-275.	2.3	236
131	Hydrophobic Compounds Reshape Membrane Domains. PLoS Computational Biology, 2014, 10, e1003873.	1.5	58
132	A conceptual modelling for combining potentials in both coarse grain and fine grain sugar molecules. , 2014, , .		1
133	Simulation of polyethylene glycol and calcium-mediated membrane fusion. Journal of Chemical Physics, 2014, 140, 124905.	1.2	44
134	Adaptive resolution simulation of an atomistic protein in MARTINI water. Journal of Chemical Physics, 2014, 140, 054114.	1.2	74
135	Computationally designed libraries for rapid enzyme stabilization. Protein Engineering, Design and Selection, 2014, 27, 49-58.	1.0	205
136	Mechanisms shaping cell membranes. Current Opinion in Cell Biology, 2014, 29, 53-60.	2.6	205
137	The power of coarse graining in biomolecular simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 225-248.	6.2	423
138	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.	7.0	77
139	Going Backward: A Flexible Geometric Approach to Reverse Transformation from Coarse Grained to Atomistic Models. Journal of Chemical Theory and Computation, 2014, 10, 676-690.	2.3	566
140	Establishing conditions for simulating hydrophobic solutes in electric fields by molecular dynamics. Journal of Molecular Modeling, 2014, 20, 2359.	0.8	2
141	Computational Library Design for Increasing Haloalkane Dehalogenase Stability. ChemBioChem, 2014, 15, 1660-1672.	1.3	68
142	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, 17170-17175.	3.3	63
143	Lipid Organization of the Plasma Membrane. Journal of the American Chemical Society, 2014, 136, 14554-14559.	6.6	734
144	Phytochemicals Perturb Membranes and Promiscuously Alter Protein Function. ACS Chemical Biology, 2014, 9, 1788-1798.	1.6	241

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145	Disaccharides Impact the Lateral Organization of Lipid Membranes. Journal of the American Chemical Society, 2014, 136, 16167-16175.	6.6	55
146	Computationally Efficient and Accurate Enantioselectivity Modeling by Clusters of Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2014, 54, 2079-2092.	2.5	44
147	The activation mode of the mechanosensitive ion channel, MscL, by lysophosphatidylcholine differs from tensionâ€induced gating. FASEB Journal, 2014, 28, 4292-4302.	0.2	42
148	Adaptive Resolution Simulation of MARTINI Solvents. Journal of Chemical Theory and Computation, 2014, 10, 2591-2598.	2.3	46
149	Perspective on the Martini model. Chemical Society Reviews, 2013, 42, 6801.	18.7	1,008
150	Defined lipid analogues induce transient channels to facilitate drug-membrane traversal and circumvent cancer therapy resistance. Scientific Reports, 2013, 3, 1949.	1.6	22
151	Interbilayer repulsion forces between tension-free lipid bilayers from simulation. Soft Matter, 2013, 9, 10705.	1.2	22
152	Coarse-grain modelling of proteinâ€“protein interactions. Current Opinion in Structural Biology, 2013, 23, 878-886.	2.6	124
153	Identification of cardiolipin binding sites on cytochrome c oxidase at the entrance of proton channels. Scientific Reports, 2013, 3, 1263.	1.6	130
154	The Martini Coarse-Grained Force Field. Methods in Molecular Biology, 2013, 924, 533-565.	0.4	107
155	Improved Parameters for the Martini Coarse-Grained Protein Force Field. Journal of Chemical Theory and Computation, 2013, 9, 687-697.	2.3	1,181
156	Mixing MARTINI: Electrostatic Coupling in Hybrid Atomisticâ€“Coarse-Grained Biomolecular Simulations. Journal of Physical Chemistry B, 2013, 117, 3516-3530.	1.2	145
157	Martini Force Field Parameters for Glycolipids. Journal of Chemical Theory and Computation, 2013, 9, 1694-1708.	2.3	166
158	Semiconducting Singleâ€Walled Carbon Nanotubes on Demand by Polymer Wrapping. Advanced Materials, 2013, 25, 2948-2956.	11.1	177
159	Improved Angle Potentials for Coarse-Grained Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 3282-3292.	2.3	67
160	Vibrational Spectra of a Mechanosensitive Channel. Journal of Physical Chemistry Letters, 2013, 4, 448-452.	2.1	22
161	Computational microscopy of cyclodextrin mediated cholesterol extraction from lipid model membranes. Scientific Reports, 2013, 3, 2071.	1.6	101
162	MARTINI Model for Physisorption of Organic Molecules on Graphite. Journal of Physical Chemistry C, 2013, 117, 15623-15631.	1.5	39

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163	Evidence for Cardiolipin Binding Sites on the Membrane-Exposed Surface of the Cytochrome bc₁. Journal of the American Chemical Society, 2013, 135, 3112-3120.	6.6	146
164	Molecular view on protein sorting into liquid-ordered membrane domains mediated by gangliosides and lipid anchors. Faraday Discussions, 2013, 161, 347-363.	1.6	76
165	Gaussian curvature elasticity determined from global shape transformations and local stress distributions: a comparative study using the MARTINI model. Faraday Discussions, 2013, 161, 365-382.	1.6	92
166	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.	1.2	3
167	Dual Action of BPC194: A Membrane Active Peptide Killing Bacterial Cells. PLoS ONE, 2013, 8, e61541.	1.1	13
168	Structural Investigation of MscL Gating Using Experimental Data and Coarse Grained MD Simulations. PLoS Computational Biology, 2012, 8, e1002683.	1.5	50
169	GPU-SD and DPD parallelization for Gromacs tools for molecular dynamics simulations. , 2012, , .		4
170	Molecular Plasticity Regulates Oligomerization and Cytotoxicity of the Multipeptide-length Amyloid-Î² Peptide Pool. Journal of Biological Chemistry, 2012, 287, 36732-36743.	1.6	37
171	Mixing Martinis: Atomistic Simulations of MscL in a Coarse Grained Environment. Biophysical Journal, 2012, 102, 241a.	0.2	0
172	Probing the Receptor Dimer Interfaces of G-Protein Coupled Receptor in Model Membranes. Biophysical Journal, 2012, 102, 515a-516a.	0.2	0
173	Rhodopsin Forms a Dimer with Cytoplasmic Helix 8 Contacts in Native Membranes. Biochemistry, 2012, 51, 1819-1821.	1.2	65
174	Efficient Algorithms for Langevin and DPD Dynamics. Journal of Chemical Theory and Computation, 2012, 8, 3637-3649.	2.3	243
175	Transmembrane helices can induce domain formation in crowded model membranes. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 984-994.	1.4	113
176	Dimerization of Amino Acid Side Chains: Lessons from the Comparison of Different Force Fields. Journal of Chemical Theory and Computation, 2012, 8, 1003-1014.	2.3	54
177	Amylose folding under the influence of lipids. Carbohydrate Research, 2012, 364, 1-7.	1.1	72
178	Structural Determinants of the Supramolecular Organization of G Protein-Coupled Receptors in Bilayers. Journal of the American Chemical Society, 2012, 134, 10959-10965.	6.6	199
179	In Silico Design of Robust Bolalipid Membranes. Biomacromolecules, 2012, 13, 196-205.	2.6	38
180	Molecular View of the Role of Fusion Peptides in Promoting Positive Membrane Curvature. Journal of the American Chemical Society, 2012, 134, 1543-1552.	6.6	74

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