

CITATION REPORT

List of articles citing

The MARTINI Coarse-Grained Force Field: Extension to Prote

DOI: 10.1021/ct700324x

Journal of Chemical Theory and Computation, 2008, 4, 819-34

Source: <https://exaly.com/paper-pdf/44040288/citation-report.pdf>

Version: 2024-04-27

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
1995	Coarse-Grained Models for Automated Fragmentation and Parametrization of Molecular Databases.		
1994	Simulation of Mixed Self-Assembled Monolayers on Gold: Effect of Terminal Alkyl Anchor Chain and Monolayer Composition.		
1993	Palmitoylation of Claudin5 Proteins Influences Their Lipid Domain Affinity and Tight Junction Assembly at the BloodBrain Barrier Interface.		
1992	Self-Assembled Nanostructures of Peptide Amphiphiles: Charge Regulation by Size Regulation.		
1991	Association of Peripheral Membrane Proteins with Membranes: Free Energy of Binding of GRP1 PH Domain with Phosphatidylinositol Phosphate-Containing Model Bilayers.		
1990	Diffusion of Integral Membrane Proteins in Protein-Rich Membranes.		
1989	Phospholipid Scramblases Remodel the Shape of Asymmetric Membranes.		
1988	Computational Investigations of the Interaction between the Cell Membrane and Nanoparticles Coated with a Pulmonary Surfactant.		
1987	Molecular Architecture of the Blood Brain Barrier Tight Junction ProteinsA Synergistic Computational and In Vitro Approach.		
1986	Testing High Concentrations of Membrane Active Antibiotic Chlorhexidine Via Computational Titration and Calorimetry.		
1985	Arbitrary Resolution with Two Bead Types Coarse-Grained Strategy and Applications to Protein Recognition.		
1984	It Is Complicated: Curvature, Diffusion, and Lipid Sorting within the Two Membranes of Escherichia coli.		
1983	Biocatalytic Self-Assembly of Tripeptide Gels and Emulsions.		
1982	Expanding the Nanoarchitectural Diversity Through Aromatic Di- and Tri-Peptide Coassembly: Nanostructures and Molecular Mechanisms.		
1981	Osmolyte Induced Changes in Peptide Conformational Ensemble Correlate with Slower Amyloid Aggregation: A Coarse-Grained Simulation Study.		
1980	Analysis of Lipid Order States and Domains in Lipid Bilayer Simulations.		
1979	.		

1978	Large-scale molecular dynamics simulations of self-assembling systems. 2008 , 321, 798-800	336
1977	CGDB: a database of membrane protein/lipid interactions by coarse-grained molecular dynamics simulations. 2008 , 25, 662-9	36
1976	DNA and lipid bilayers: self-assembly and insertion. 2008 , 5 Suppl 3, S241-50	59
1975	Computer simulation study of fullerene translocation through lipid membranes. 2008 , 3, 363-8	411
1974	Multiscale methods for macromolecular simulations. 2008 , 18, 630-40	169
1973	Coarse-grained molecular dynamics simulations of the energetics of helix insertion into a lipid bilayer. 2008 , 47, 11321-31	85
1972	Distribution of amino acids in a lipid bilayer from computer simulations. 2008 , 94, 3393-404	434
1971	The interaction of phospholipase A2 with a phospholipid bilayer: coarse-grained molecular dynamics simulations. 2008 , 95, 1649-57	38
1970	Coarse-grained simulations of the membrane-active antimicrobial Peptide maculatin 1.1. 2008 , 95, 3802-15	61
1969	Lipid bilayer deformation and the free energy of interaction of a Kv channel gating-modifier toxin. 2008 , 95, 3816-26	26
1968	Self-assembly of a simple membrane protein: coarse-grained molecular dynamics simulations of the influenza M2 channel. 2008 , 95, 3790-801	67
1967	Coarse-grained simulation studies of peptide-induced pore formation. 2008 , 95, 4163-73	59
1966	Peptide aggregation and pore formation in a lipid bilayer: a combined coarse-grained and all atom molecular dynamics study. 2008 , 95, 4337-47	113
1965	Toward a Coarse-Grained Protein Model Coupled with a Coarse-Grained Solvent Model: Solvation Free Energies of Amino Acid Side Chains. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 1891-901 ^{6.4}	31
1964	Lipid bilayer curvature and pore formation induced by charged linear polymers and dendrimers: the effect of molecular shape. 2008 , 112, 12279-85	100
1963	Topologically Based Multipolar Reconstruction of Electrostatic Interactions in Multiscale Simulations of Proteins. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 1378-85	6.4 24
1962	Hierarchical structure controls nanomechanical properties of vimentin intermediate filaments. 2009 , 4, e7294	129
1961	Molecular Dynamics Computations for Proteins: A Case Study in Membrane Ion Permeation. 2009 ,	

1960	The multiscale coarse-graining method. III. A test of pairwise additivity of the coarse-grained potential and of new basis functions for the variational calculation. 2009 , 131, 034102	50
1959	Solving the equations of motion for mixed atomistic and coarse-grained systems. 2009 , 35, 962-973	25
1958	Coarse-grained ions without charges: reproducing the solvation structure of NaCl in water using short-ranged potentials. 2009 , 131, 034107	61
1957	Simulations of the c-subunit of ATP-synthase reveal helix rearrangements. 2009 , 26, 422-34	22
1956	Extended ensemble approach for deriving transferable coarse-grained potentials. 2009 , 131, 104110	87
1955	Systematic coarse graining from structure using internal states: application to phospholipid/cholesterol bilayer. 2009 , 131, 055101	49
1954	The multiscale coarse-graining method. IV. Transferring coarse-grained potentials between temperatures. 2009 , 131, 024103	95
1953	Maturation of high-density lipoproteins. 2009 , 6, 863-71	36
1952	Systematic multiscale simulation of membrane protein systems. 2009 , 19, 138-44	87
1951	Long-timescale molecular dynamics simulations of protein structure and function. 2009 , 19, 120-7	562
1950	Coarse-grain simulations of the R-SNARE fusion protein in its membrane environment detect long-lived conformational sub-states. 2009 , 10, 1548-52	27
1949	RedMD--reduced molecular dynamics package. 2009 , 30, 2364-73	18
1948	From fast light-activated processes in biomolecules to large-scale aggregation of membrane proteins: molecular dynamics simulations at different time and length scales. 2009 , 3,	
1947	The structural basis for peptide selection by the transport receptor OppA. 2009 , 28, 1332-40	66
1946	Self assembly of peptides near or within membranes using coarse grained MD simulations. 2009 , 358, 161-170	27
1945	Coarse-grained modeling of lipids. 2009 , 159, 59-66	75
1944	Effects of carbon nanoparticles on lipid membranes: a molecular simulation perspective. 2009 , 5, 4433	94
1943	The interaction of C60 and its derivatives with a lipid bilayer via molecular dynamics simulations. 2009 , 20, 115102	68

1942	A Transferable Coarse Grain Non-bonded Interaction Model For Amino Acids. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 2115-2124	6.4	106
1941	PIP(2)-binding site in Kir channels: definition by multiscale biomolecular simulations. 2009 , 48, 10926-33		108
1940	Charge equilibration force fields for lipid environments: applications to fully hydrated DPPC bilayers and DMPC-embedded gramicidin A. 2009 , 113, 9183-96		40
1939	Dynamics of activation of lecithin:cholesterol acyltransferase by apolipoprotein A-I. 2009 , 48, 11196-210		38
1938	An improved functional form for the temperature scaling factors of the components of the mesoscopic UNRES force field for simulations of protein structure and dynamics. 2009 , 113, 8738-44		37
1937	Hybrid coarse-graining approach for lipid bilayers at large length and time scales. 2009 , 113, 4413-24		52
1936	Coarse Point Charge Models For Proteins From Smoothed Molecular Electrostatic Potentials. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 3279-98	6.4	11
1935	Alamethicin in lipid bilayers: combined use of X-ray scattering and MD simulations. 2009 , 1788, 1387-97		85
1934	Ectodomain orientation, conformational plasticity and oligomerization of ErbB1 receptors investigated by molecular dynamics. 2009 , 167, 117-28		39
1933	Insights from coarse-grained G Γ models for protein folding and dynamics. 2009 , 10, 889-905		198
1932	Generic coarse-grained model for protein folding and aggregation. 2009 , 130, 235106		155
1931	Molecular dynamics simulations of a DMPC bilayer using nonadditive interaction models. 2009 , 96, 385-402		52
1930	Lipid gymnastics: evidence of complete acyl chain reversal in oxidized phospholipids from molecular simulations. 2009 , 96, 2734-43		109
1929	Peptide nanopores and lipid bilayers: interactions by coarse-grained molecular-dynamics simulations. 2009 , 96, 3519-28		25
1928	Curvature generation and pressure profile modulation in membrane by lysolipids: insights from coarse-grained simulations. 2009 , 97, 2267-76		60
1927	Hybrid particle-field molecular dynamics simulations for dense polymer systems. 2009 , 130, 214106		83
1926	Combining an Elastic Network With a Coarse-Grained Molecular Force Field: Structure, Dynamics, and Intermolecular Recognition. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 2531-43	6.4	397
1925	Molecular Theory Applied to Lipid Bilayers and LipidProtein Interactions. 2009 , 1-39		

1924	Coarse-grained molecular dynamics simulation of ammonium surfactant self-assemblies: micelles and vesicles. 2009 , 113, 15010-6		49
1923	Coarse-grained molecular dynamics study of cyclic peptide nanotube insertion into a lipid bilayer. 2009 , 113, 4780-7		34
1922	Martini Coarse-Grained Force Field: Extension to Carbohydrates. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 3195-210	6.4	302
1921	Coarse-Grained MD Simulations and Protein-Protein Interactions: The Cohesin-Dockerin System. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 2465-71	6.4	25
1920	Multiscale simulation of soft matter systems IFrom the atomistic to the coarse-grained level and back. 2009 , 5, 4357		342
1919	Interaction of monotopic membrane enzymes with a lipid bilayer: a coarse-grained MD simulation study. 2009 , 48, 2135-45		39
1918	Multiscale modeling of emergent materials: biological and soft matter. 2009 , 11, 1869-92		217
1917	Developing Coarse-Grained Force Fields for PNIPAM Single Chain from the Atomistic Model. 2009 ,		1
1916	Spontaneous formation of a barrel-stave pore in a coarse-grained model of the synthetic LS3 peptide and a DPPC lipid bilayer. 2009 , 113, 6-8		21
1915	Self-assembling dipeptides: conformational sampling in solvent-free coarse-grained simulation. 2009 , 11, 2077-86		73
1914	On using a too large integration time step in molecular dynamics simulations of coarse-grained molecular models. 2009 , 11, 1934-41		70
1913	Self-assembling dipeptides: including solvent degrees of freedom in a coarse-grained model. 2009 , 11, 2068-76		51
1912	Exploring gas permeability of lipid membranes using coarse-grained molecular dynamics. 2009 , 35, 953-961		13
1911	3D pressure field in lipid membranes and membrane-protein complexes. 2009 , 102, 078101		156
1910	A coarse-grained model for polyethylene oxide and polyethylene glycol: conformation and hydrodynamics. 2009 , 113, 13186-94		298
1909	A single bicontinuous cubic phase induced by fusion peptides. 2009 , 131, 9166-7		44
1908	Location, tilt, and binding: a molecular dynamics study of voltage-sensitive dyes in biomembranes. 2009 , 113, 15807-19		31
1907	Pressure calculation in hybrid particle-field simulations. 2010 , 133, 214102		34

1906	Defect-mediated trafficking across cell membranes: insights from in silico modeling. 2010 , 110, 6077-103	153
1905	QM/MM methods: looking inside heme proteins biochemistry. 2010 , 149, 1-11	34
1904	How to predict diffusion of medium-sized molecules in polymer matrices. From atomistic to coarse grain simulations. 2010 , 16, 1845-51	25
1903	The structure of the talin/integrin complex at a lipid bilayer: an NMR and MD simulation study. 2010 , 18, 1280-8	53
1902	Reconstruction of atomistic details from coarse-grained structures. 2010 , 31, 1333-43	127
1901	Characterization of a clinical polymer-drug conjugate using multiscale modeling. 2010 , 93, 936-51	19
1900	PRIMO/PRIMONA: a coarse-grained model for proteins and nucleic acids that preserves near-atomistic accuracy. 2010 , 78, 1266-81	78
1899	Molecular Simulation Methods. 2010 , 155-178	1
1898	Polarizable water model for the coarse-grained MARTINI force field. 2010 , 6, e1000810	587
1897	Release of content through mechano-sensitive gates in pressurized liposomes. 2010 , 107, 19856-60	99
1896	Assessment of the validity of the double superhelix model for reconstituted high density lipoproteins: a combined computational-experimental approach. 2010 , 285, 41161-71	50
1895	Structural evolution of protein-biofilms: Simulations and experiments. 2010 , 4, 32201	20
1894	The multiscale coarse-graining method. V. Isothermal-isobaric ensemble. 2010 , 132, 164106	98
1893	The multiscale coarse-graining method: assessing its accuracy and introducing density dependent coarse-grain potentials. 2010 , 133, 064109	75
1892	Immobilization of the plug domain inside the SecY channel allows unrestricted protein translocation. 2010 , 285, 23747-54	25
1891	Coarse grained molecular dynamics simulations of transmembrane protein-lipid systems. 2010 , 11, 2393-420	21
1890	Role of lipids in spheroidal high density lipoproteins. 2010 , 6, e1000964	69
1889	Composition and lipid spatial distribution of HDL particles in subjects with low and high HDL-cholesterol. 2010 , 51, 2341-51	93

1888	Multiscale coarse-graining of the protein energy landscape. 2010 , 6, e1000827		101
1887	The role of oligomerization and cooperative regulation in protein function: the case of tryptophan synthase. 2010 , 6, e1000994		31
1886	Coarse-grained models to study dynamics of nanoscale biomolecules and their applications to the ribosome. 2010 , 22, 453101		30
1885	Stretched exponential dynamics in lipid bilayer simulations. 2010 , 133, 115101		22
1884	Reference state for the generalized Yvon-Born-Green theory: application for coarse-grained model of hydrophobic hydration. 2010 , 133, 124107		21
1883	Molecular dynamics of membrane peptides and proteins: principles and comparison to experimental data. 2010 , 654, 403-21		4
1882	On the antibacterial action of cyclic peptides: insights from coarse-grained MD simulations. 2010 , 114, 2676-84		39
1881	Molecular dynamics simulation of protein adsorption at fluid interfaces: a comparison of all-atom and coarse-grained models. 2010 , 11, 2781-7		24
1880	Many-body interactions and coarse-grained simulations of structure of nanoparticle-polymer melt mixtures. 2010 , 133, 144904		28
1879	A Coarse-Grained Model Based on Morse Potential for Water and n-Alkanes. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 851-63	6.4	61
1878	Membrane/Toxin Interaction Energetics via Serial Multiscale Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 966-76	6.4	14
1877	Multiscale simulation of soft matter systems. 2010 , 144, 9-24		141
1876	Interactions between a voltage sensor and a toxin via multiscale simulations. 2010 , 98, 1558-65		24
1875	Lipid-modulated sequence-specific association of glycophorin A in membranes. 2010 , 99, 284-92		49
1874	Interpretation of 2H-NMR experiments on the orientation of the transmembrane helix WALP23 by computer simulations. 2010 , 99, 1455-64		41
1873	Influence of hydrophobic mismatch and amino acid composition on the lateral diffusion of transmembrane peptides. 2010 , 99, 1447-54		72
1872	Direct simulation of protein-mediated vesicle fusion: lung surfactant protein B. 2010 , 99, 2134-42		64
1871	The energetics of transmembrane helix insertion into a lipid bilayer. 2010 , 99, 2534-40		20

1870	Multiscale computer simulation of the immature HIV-1 virion. 2010 , 99, 2757-65		63
1869	Functional modes and residue flexibility control the anisotropic response of guanylate kinase to mechanical stress. 2010 , 99, 3412-9		19
1868	Self-association of models of transmembrane domains of ErbB receptors in a lipid bilayer. 2010 , 99, 3657-65		38
1867	Membrane poration by antimicrobial peptides combining atomistic and coarse-grained descriptions. 2010 , 144, 431-43; discussion 445-81		112
1866	A systematically coarse-grained solvent-free model for quantitative phospholipid bilayer simulations. 2010 , 114, 11207-20		116
1865	A Generalized-YvonBornGreen Theory for Determining Coarse-Grained Interaction Potentials		78
1864	PACE Force Field for Protein Simulations. 2. Folding Simulations of Peptides. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 3390-402	6.4	39
1863	Lessons from free energy simulations of delta-opioid receptor homodimers involving the fourth transmembrane helix. 2010 , 49, 6771-6		42
1862	A new coarse-grained model for water: the importance of electrostatic interactions. 2010 , 114, 10524-9		150
1861	What Is the Difference Between a Supported and a Free Bilayer? Insights from Molecular Modeling on Different Scales. 2010 , 11, 127-157		2
1860	Changes in transmembrane helix alignment by arginine residues revealed by solid-state NMR experiments and coarse-grained MD simulations. 2010 , 132, 5803-11		69
1859	Coarse grained simulations of local anesthetics encapsulated into a liposome. 2010 , 114, 7009-15		13
1858	PACE Force Field for Protein Simulations. 1. Full Parameterization of Version 1 and Verification. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 3373-89	6.4	57
1857	Coarse-Grained Model of Collagen Molecules Using an Extended MARTINI Force Field. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 1210-1218	6.4	80
1856	Mechanism of substrate shuttling by the acyl-carrier protein within the fatty acid mega-synthase. 2010 , 132, 12357-64		29
1855	Molecular dynamics simulations of the dimerization of transmembrane alpha-helices. 2010 , 43, 388-96		72
1854	Multiscale modeling of proteins. 2010 , 43, 220-30		111
1853	Coarse-grained models: getting more with less. 2010 , 10, 753-9		23

1852	Folding of lipid monolayers containing lung surfactant proteins SP-B(1-25) and SP-C studied via coarse-grained molecular dynamics simulations. 2010 , 1798, 1632-50		33
1851	Antimicrobial Peptides Induce Growth of Phosphatidylglycerol Domains in a Model Bacterial Membrane. 2010 , 1, 3108-3111		56
1850	Efficient, Regularized, and Scalable Algorithms for Multiscale Coarse-Graining. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 954-65	6.4	95
1849	Membrane proteins diffuse as dynamic complexes with lipids. 2010 , 132, 7574-5		140
1848	Penetration of lipid membranes by gold nanoparticles: insights into cellular uptake, cytotoxicity, and their relationship. 2010 , 4, 5421-9		479
1847	Lipid-mediated interactions tune the association of glycoporphin A helix and its disruptive mutants in membranes. 2010 , 12, 12987-96		93
1846	Membrane protein dynamics from femtoseconds to seconds. 2010 , 654, 423-40		9
1845	Minimalist models for proteins: a comparative analysis. 2010 , 43, 333-71		87
1844	Lipidomics. 2010 ,		
1843	Coarse-grained potential models for phenyl-based molecules: I. Parametrization using experimental data. 2010 , 114, 6386-93		49
1842	Membrane Protein Structure Determination. 2010 ,		4
1841	Protein Backbone Dynamics Simulations Using Coarse-Grained Bonded Potentials and Simplified Hydrogen Bonds. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 761-73	6.4	19
1840	Interactions of phospholipid bilayers with several classes of amphiphilic alpha-helical peptides: insights from coarse-grained molecular dynamics simulations. 2010 , 114, 826-39		47
1839	Diffusion of gases across lipid membranes with OmpA channel: a molecular dynamics study. 2010 , 108, 1569-1581		12
1838	Coarse-Grained Model for Perfluorocarbons and Phase Equilibrium Simulation of Perfluorocarbons/CO ₂ Mixtures. 2010 , 49, 8271-8278		9
1837	Bioinspired noncovalently crosslinked fuzzy carbon nanotube bundles with superior toughness and strength. 2010 , 20, 10465		36
1836	A simple coarse-grained model for self-assembling silk-like protein fibers. 2010 , 144, 127-41; discussion 203-22, 467-81		8
1835	A Nonradial Coarse-Grained Potential for Proteins Produces Naturally Stable Secondary Structure Elements. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 315-24	6.4	42

1834	Lateral pressure profiles in lipid monolayers. 2010 , 144, 393-409; discussion 445-81	46
1833	Colloquium: Failure of molecules, bones, and the Earth itself. 2010 , 82, 1459-1487	36
1832	Permeation of nanocrystals across lipid membranes. 2011 , 109, 1511-1526	30
1831	Protofibrillar Assembly Toward the Formation of Amyloid Fibrils. 2011 , 2, 2385-2390	34
1830	Molecular modeling of the human serotonin(1A) receptor: role of membrane cholesterol in ligand binding of the receptor. 2011 , 7, 224-34	55
1829	Multiscale modelling of mesoscopic phenomena triggered by quantum events: light-driven azo-materials and beyond. 2011 , 13, 7604-21	48
1828	Assessing the Quality of the OPEP Coarse-Grained Force Field. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 1928-34	6.4 25
1827	Virtual Screening for Dipeptide Aggregation: Toward Predictive Tools for Peptide Self-Assembly. 2011 , 2, 2380-2384	129
1826	Synaptotagmin-1 may be a distance regulator acting upstream of SNARE nucleation. 2011 , 18, 805-12	98
1825	Coarse-grained molecular dynamics simulations of the sphere to rod transition in surfactant micelles. 2011 , 27, 6628-38	112
1824	pyDockCG: new coarse-grained potential for protein-protein docking. 2011 , 115, 6032-9	14
1823	Implementation of a protein reduced point charge model toward molecular dynamics applications. 2011 , 115, 12531-43	3
1822	Structure and phase transformations of DPPC lipid bilayers in the presence of nanoparticles: insights from coarse-grained molecular dynamics simulations. 2011 , 27, 3723-30	74
1821	Exploration of transferability in multiscale coarse-grained peptide models. 2011 , 115, 11911-26	20
1820	Spontaneous buckling of lipid bilayer and vesicle budding induced by antimicrobial peptide magainin 2: a coarse-grained simulation study. 2011 , 115, 8122-9	58
1819	Interaction of diverse voltage sensor homologs with lipid bilayers revealed by self-assembly simulations. 2011 , 100, 875-84	11
1818	Membrane insertion of a voltage sensor helix. 2011 , 100, 410-9	14
1817	Lung surfactant protein SP-B promotes formation of bilayer reservoirs from monolayer and lipid transfer between the interface and subphase. 2011 , 100, 1678-87	49

1816	Protein shape change has a major effect on the gating energy of a mechanosensitive channel. 2011 , 100, 1651-9	45
1815	Exploring peptide-membrane interactions with coarse-grained MD simulations. 2011 , 100, 1940-8	39
1814	Aggregation of model membrane proteins, modulated by hydrophobic mismatch, membrane curvature, and protein class. 2011 , 101, 691-9	101
1813	GxxxG motifs, phenylalanine, and cholesterol guide the self-association of transmembrane domains of ErbB2 receptors. 2011 , 101, 1949-58	33
1812	Aggregation properties of a polymeric anticancer therapeutic: a coarse-grained modeling study. 2011 , 51, 3030-5	8
1811	Structure and dynamics of the membrane-bound cytochrome P450 2C9. 2011 , 7, e1002152	121
1810	Coarse-grained modeling for macromolecular chemistry. 2012 , 307, 295-321	46
1809	Molecular Dynamics Studies of the Size and Internal Structure of the PAMAM Dendrimer Grafted with Arginine and Histidine. 2011 , 44, 8681-8686	26
1808	Coarse-graining entropy, forces, and structures. 2011 , 135, 214101	103
1807	Multiscale modeling of soft matter: scaling of dynamics. 2011 , 13, 10412-20	133
1806	Coarse-grained force field: general folding theory. 2011 , 13, 16890-901	63
1805	A Coarse-Grained Model for Molecular Dynamics Simulations of Native Cellulose. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 753-760	6.4 69
1804	Hybrid simulations: combining atomistic and coarse-grained force fields using virtual sites. 2011 , 13, 10437-48	153
1803	Low density lipoprotein: structure, dynamics, and interactions of apoB-100 with lipids. 2011 , 7, 8135	38
1802	All-atom and coarse-grained molecular dynamics simulations of a membrane protein stabilizing polymer. 2011 , 27, 10523-37	53
1801	Driving Force for the Association of Hydrophobic Peptides: The Importance of Electrostatic Interactions in Coarse-Grained Water Models. 2011 , 2, 1794-1798	31
1800	Ordering surfaces on the nanoscale: implications for protein adsorption. 2011 , 133, 1438-50	130
1799	Modeling the interfacial tension in oil-water-nonionic surfactant mixtures using dissipative particle dynamics and self-consistent field theory. 2011 , 115, 4654-61	57

1798	From Coarse Grained to Atomistic: A Serial Multiscale Approach to Membrane Protein Simulations. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 1157-66	6.4	200
1797	A New Coarse-Grained Force Field for Membrane-Peptide Simulations. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 3793-802	6.4	70
1796	Hybrid Particle-Field Coarse-Grained Models for Biological Phospholipids. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2947-62	6.4	48
1795	Molecular dynamics simulation of a polysorbate 80 micelle in water. 2011 , 7, 2900		57
1794	A MARTINI Coarse-Grained Model of a Thermoset Polyester Coating. 2011 , 44, 6198-6208		51
1793	Using the Wimley-White Hydrophobicity Scale as a Direct Quantitative Test of Force Fields: The MARTINI Coarse-Grained Model. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2316-24	6.4	38
1792	Molecular dynamics simulation of phase transitions in model lung surfactant monolayers. 2011 , 1808, 2450-65		55
1791	Competing interactions for antimicrobial selectivity based on charge complementarity. 2011 , 1808, 2867-76		21
1790	Making structural sense of dimerization interfaces of delta opioid receptor homodimers. 2011 , 50, 1682-90		66
1789	Chapter 21: Investigating Mechanisms of Ligand Recognition, Activation and Oligomerization in GPCRs Using Enhanced Molecular Dynamics Methods. 2011 , 401-428		
1788	A Hybrid All-Atom Structure-Based Model for Protein Folding and Large Scale Conformational Transitions. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 4208-17	6.4	19
1787	Lipid simulations: a perspective on lipids in action. 2011 , 3,		29
1786	Coarse-graining polymers with the MARTINI force-field: polystyrene as a benchmark case. 2011 , 7, 698-708		186
1785	Gap junction hemichannel interactions with zwitterionic lipid, anionic lipid, and cholesterol: molecular simulation studies. 2011 , 50, 1492-504		20
1784	Assessment of Glycoproteins Dynamics from Computer Simulations. 2011 , 8, 229-238		11
1783	Multiscale Modeling of Functionalized Nanocarriers in Targeted Drug Delivery. 2011 , 7, 727-735		28
1782	Abstracts of Albany 2011, the 17th Conversation. June 14-18 2011. Albany, New York, USA. 2011 , 28, 975-1170		1
1781	A smoothly decoupled particle interface: new methods for coupling explicit and implicit solvent. 2011 , 134, 214103		15

1780	A helix heterodimer in a lipid bilayer: prediction of the structure of an integrin transmembrane domain via multiscale simulations. 2011 , 19, 1477-84	35
1779	Molecular simulation approaches to membrane proteins. 2011 , 19, 1562-72	136
1778	Recent development in computer simulations of lipid bilayers. 2011 , 7, 25-39	122
1777	MSCALE: A General Utility for Multiscale Modeling. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 1208-1219	6.4 38
1776	Charge density distributions derived from smoothed electrostatic potential functions: design of protein reduced point charge models. 2011 , 25, 913-30	8
1775	Coarse-grained modeling study of nonpeptide RGD ligand density and PEG molecular weight on the conformation of poly(ϵ -glutamyl-glutamate) paclitaxel conjugates. 2011 , 17, 2973-87	5
1774	Fluorescence spectroscopy and molecular dynamics simulations in studies on the mechanism of membrane destabilization by antimicrobial peptides. 2011 , 68, 2281-301	42
1773	Inhibition of peptide aggregation by lipids: insights from coarse-grained molecular simulations. 2011 , 29, 597-607	16
1772	Modification of Martini force field for molecular dynamics simulation of hydrophobic charge induction chromatography of lysozyme. 2011 , 29, 906-14	17
1771	Study of the Alzheimer's A β 40 peptide in SDS micelles using molecular dynamics simulations. 2011 , 153, 179-86	9
1770	Interdomain compactization in human tyrosyl-tRNA synthetase studied by the hierarchical rotations technique. 2011 , 154, 90-8	11
1769	Mechanics of Microtubules from a Coarse-Grained Model. 2011 , 1, 173-182	7
1768	Leukocyte integrin α 2 transmembrane association dynamics revealed by coarse-grained molecular dynamics simulations. 2011 , 79, 2203-13	20
1767	A Challenge for Peptide Coarse Graining: Transferability of Fragment-Based Models. 2011 , 20, 451-465	26
1766	Coarse-Grained Simulations of Model Polymer Nanofibres. 2011 , 20, 305-319	24
1765	Hybrid Approaches to Coarse-Graining using the VOTCA Package: Liquid Hexane. 2011 , 20, 472-477	40
1764	Generalized-YvonBornGreen Model of Toluene. 2011 , 20, 478-495	18
1763	Structural, dynamic, and electrostatic properties of fully hydrated DMPC bilayers from molecular dynamics simulations accelerated with graphical processing units (GPUs). 2011 , 32, 2958-73	18

1762	DynamO: a free O(N) general event-driven molecular dynamics simulator. 2011 , 32, 3329-38	109
1761	Caught in the act: visualization of SNARE-mediated fusion events in molecular detail. 2011 , 12, 1049-55	109
1760	Coarse-grained mechanochemical model for simulating the dynamic behavior of microtubules. 2011 , 84, 031933	25
1759	Effects of cholesterol on pore formation in lipid bilayers induced by human islet amyloid polypeptide fragments: a coarse-grained molecular dynamics study. 2011 , 84, 051922	27
1758	Multiscale simulations suggest a mechanism for integrin inside-out activation. 2011 , 108, 11890-5	56
1757	A Review of Coarse-Grained Molecular Dynamics Techniques to Access Extended Spatial and Temporal Scales in Biomolecular Simulations. 2011 , 67-87	26
1756	Nanocomputation of Mechanical Properties in Nanobio Membrane. 2011 , 110-116, 3883-3887	
1755	Lipid packing drives the segregation of transmembrane helices into disordered lipid domains in model membranes. 2011 , 108, 1343-8	193
1754	Coarse-Grained Molecular Dynamics Simulation of Lysozyme Protein Crystals. 2011 , 6,	1
1753	Transmembrane helix dynamics of bacterial chemoreceptors supports a piston model of signalling. 2011 , 7, e1002204	34
1752	Mechanism of bacterial signal transduction revealed by molecular dynamics of Tsr dimers and trimers of dimers in lipid vesicles. 2012 , 8, e1002685	34
1751	Structural insights into the inhibition of actin-capping protein by interactions with phosphatidic acid and phosphatidylinositol (4,5)-bisphosphate. 2012 , 8, e1002765	40
1750	Structural investigation of MscL gating using experimental data and coarse grained MD simulations. 2012 , 8, e1002683	37
1749	Phase Behavior of a Lipid Bilayer System Studied by a Replica-Exchange Molecular Dynamics Simulation. 2012 , 81, 024002	16
1748	Role of surface ligands in nanoparticle permeation through a model membrane: a coarse-grained molecular dynamics simulations study. 2012 , 110, 2181-2195	28
1747	Charge localization in multiply charged clusters and their electrical properties: some insights into electrostatic droplets. 2012 , 136, 184503	7
1746	The multiscale coarse-graining method. X. Improved algorithms for constructing coarse-grained potentials for molecular systems. 2012 , 136, 194115	37
1745	The multiscale coarse-graining method. IX. A general method for construction of three body coarse-grained force fields. 2012 , 136, 194114	47

1744	The multiscale coarse-graining method. VIII. Multiresolution hierarchical basis functions and basis function selection in the construction of coarse-grained force fields. 2012 , 136, 194113	19
1743	Effect of secondary structure on the self-assembly of amphiphilic molecules: a multiscale simulation study. 2012 , 136, 084902	11
1742	Structure of saposin A lipoprotein discs. 2012 , 109, 2908-12	61
1741	Multiscale Modeling for Host-Guest Chemistry of Dendrimers in Solution. 2012 , 4, 463-485	14
1740	Structure-based coarse-graining in liquid slabs. 2012 , 137, 064102	38
1739	Recent advances in computational modeling of helical membrane-active peptides. 2012 , 13, 644-57	18
1738	- Nucleation and Crystalline Growth Kinetics. 2012 , 46-119	
1737	Challenges in analysing and visualizing large-scale molecular dynamics simulations: domain and defect formation in lung surfactant monolayers. 2012 , 385, 012002	2
1736	Interfacial tension and surface pressure of high density lipoprotein, low density lipoprotein, and related lipid droplets. 2012 , 103, 1236-44	30
1735	Peptide nanovesicles formed by the self-assembly of branched amphiphilic peptides. 2012 , 7, e45374	65
1734	Further optimization of a hybrid united-atom and coarse-grained force field for folding simulations: Improved backbone hydration and interactions between charged side chains. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 4413-4424	6.4 95
1733	Thirty-five years of biomolecular simulation: development of methodology, force fields and software. 2012 , 38, 1271-1281	18
1732	Coarse-grain simulations reveal movement of the synaptobrevin C-terminus in response to piconewton forces. 2012 , 103, 959-69	37
1731	A generic force field for protein coarse-grained molecular dynamics simulation. 2012 , 13, 14451-69	14
1730	Peptide-lipid interactions of the stress-response peptide TisB that induces bacterial persistence. 2012 , 103, 1460-9	39
1729	Molecular simulation of hydrophobin adsorption at an oil-water interface. 2012 , 28, 8730-6	49
1728	Adsorption of Proteins onto Ion-Exchange Chromatographic Media: A Molecular Dynamics Study. 2012 , 51, 16049-16058	16
1727	Molecular dynamics simulations of creatine kinase and adenine nucleotide translocase in mitochondrial membrane patch. 2012 , 287, 7467-76	18

1726	Peptide chain dynamics in light and heavy water: zooming in on internal friction. 2012 , 134, 6273-9		76
1725	Multi-layer coarse-graining polarization model for treating electrostatic interactions of solvated β -onotoxin peptides. 2012 , 136, 134105		11
1724	Multi-scale simulation of the simian immunodeficiency virus fusion peptide. 2012 , 116, 13713-21		10
1723	Cholesterol modulates the structure, binding modes, and energetics of caveolin-membrane interactions. 2012 , 116, 14556-64		30
1722	Molecular Dynamics Study of a MARTINI Coarse-Grained Polystyrene Brush in Good Solvent: Structure and Dynamics. 2012 , 45, 563-571		28
1721	Identification of cholesterol binding sites in the serotonin1A receptor. 2012 , 116, 12991-6		113
1720	β Synuclein induces both positive mean curvature and negative Gaussian curvature in membranes. 2012 , 134, 2613-20		88
1719	Probing the self-assembly mechanism of diphenylalanine-based peptide nanovesicles and nanotubes. 2012 , 6, 3907-18		213
1718	The coarse-grained OPEP force field for non-amyloid and amyloid proteins. 2012 , 116, 8741-52		80
1717	Molecular crystallization controlled by pH regulates mesoscopic membrane morphology. 2012 , 6, 10901-9		43
1716	The Transmembrane Helix Tilt May Be Determined by the Balance between Precession Entropy and Lipid Perturbation. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 2896-2904	6.4	11
1715	Multifaceted substrate capture scheme of a rhomboid protease. 2012 , 116, 8942-54		22
1714	Accommodation of a central arginine in a transmembrane peptide by changing the placement of anchor residues. 2012 , 116, 12980-90		21
1713	Derivation of coarse grained models for multiscale simulation of liquid crystalline phase transitions. 2012 , 116, 8474-84		58
1712	Tunable, mixed-resolution modeling using library-based Monte Carlo and graphics processing units. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 2921-2929	6.4	10
1711	Coarse-Graining Approach to Infer Mesoscale Interaction Potentials from Atomistic Interactions for Aggregating Systems. 2012 , 51, 16116-16134		6
1710	Formation and domain partitioning of H-ras peptide nanoclusters: effects of peptide concentration and lipid composition. 2012 , 134, 17278-85		50
1709	Assessment of Atomic Charge Models for Gas-Phase Computations on Polypeptides. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 661-76	6.4	60

1708	Effects of the Size, Shape, and Structural Transition of Thermosensitive Polypeptides on the Stability of Lipid Bilayers and Liposomes. 2012 , 45, 7304-7312		16
1707	Suitability of the MARTINI Force Field for Use with Gas-Phase Protein Complexes. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1304-13	6.4	11
1706	REACH coarse-grained simulation of a cellulose fiber. 2012 , 13, 2634-44		30
1705	Modeling the self-assembly of peptide amphiphiles into fibers using coarse-grained molecular dynamics. 2012 , 12, 4907-13		112
1704	A Local Rigid Body Framework for Global Optimization of Biomolecules. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 5159-65	6.4	32
1703	The role of molecular simulations in the development of inhibitors of amyloid β -peptide aggregation for the treatment of Alzheimer's disease. 2012 , 3, 845-56		85
1702	Modeling and simulation of ion channels. 2012 , 112, 6250-84		159
1701	Coarse-grained simulations of transitions in the E2-to-E1 conformations for Ca ATPase (SERCA) show entropy-enthalpy compensation. 2012 , 422, 575-93		13
1700	Transmembrane helices can induce domain formation in crowded model membranes. 2012 , 1818, 984-94		102
1699	Comparative molecular dynamics simulations of the antimicrobial peptide CM15 in model lipid bilayers. 2012 , 1818, 1402-9		63
1698	Antimicrobial selectivity based on zwitterionic lipids and underlying balance of interactions. 2012 , 1818, 2192-201		20
1697	How cholesterol is distributed between monolayers in asymmetric lipid membranes. 2012 , 41, 1043-54		31
1696	A tightly regulated molecular toggle controls AAA+ disaggregase. 2012 , 19, 1338-46		102
1695	5.16 Computer Simulation of Membrane Dynamics. 2012 , 312-336		3
1694	Dimerization of Amino Acid Side Chains: Lessons from the Comparison of Different Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1003-14	6.4	49
1693	DPD Simulation of Protein Conformations: From β -Helices to β -Structures. 2012 , 3, 3081-7		53
1692	Adsorption of unstructured protein β -casein to hydrophobic and charged surfaces. 2012 , 28, 11843-9		51
1691	Hydrophobic mismatch and lipid sorting near OmpA in mixed bilayers: atomistic and coarse-grained simulations. 2012 , 102, 2279-87		15

1690	Robust driving forces for transmembrane helix packing. 2012 , 103, 1227-35		19
1689	9.6 New Technologies for Molecular Dynamics Simulations. 2012 , 86-104		3
1688	A coarse-grained MARTINI model of polyethylene glycol and of polyoxyethylene alkyl ether surfactants. 2012 , 116, 14353-62		75
1687	Local Lipid Reorganization by a Transmembrane Protein Domain. 2012 , 3, 3498-502		28
1686	Chapter 9:Coarse-grain Protein Models. 2012 , 219-248		1
1685	The role of many-body correlations in determining potentials for coarse-grained models of equilibrium structure. 2012 , 116, 8621-35		36
1684	Exploring the dynamics of four RNA-dependent RNA polymerases by a coarse-grained model. 2012 , 116, 14515-24		16
1683	The Role of Atomic Polarization in the Thermodynamics of Chloroform Partitioning to Lipid Bilayers. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 618-28	6.4	42
1682	Parameterization of PACE Force Field for Membrane Environment and Simulation of Helical Peptides and Helix-Helix Association. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 300-13	6.4	44
1681	Insights into the endosomal escape mechanism via investigation of dendrimer-membrane interactions. 2012 , 8, 6378		66
1680	Nanoparticle permeation induces water penetration, ion transport, and lipid flip-flop. 2012 , 28, 16989-7000		34
1679	Coarse-Grained Modeling of Polystyrene in Various Environments by Iterative Boltzmann Inversion. 2012 , 45, 9205-9219		59
1678	Effects of solution concentration on the physicochemical properties of a polymeric anticancer therapeutic. 2012 , 9, 37-47		2
1677	Motion planning algorithms for molecular simulations: A survey. 2012 , 6, 125-143		56
1676	Multiscale simulations of the antimicrobial peptide maculatin 1.1: water permeation through disordered aggregates. 2012 , 116, 8485-93		27
1675	Structural determinants of the supramolecular organization of G protein-coupled receptors in bilayers. 2012 , 134, 10959-65		181
1674	Contributions to membrane-embedded-protein diffusion beyond hydrodynamic theories. 2012 , 85, 061921		29
1673	Molecular view of the role of fusion peptides in promoting positive membrane curvature. 2012 , 134, 1543-52		67

1672	Difference between magainin-2 and melittin assemblies in phosphatidylcholine bilayers: results from coarse-grained simulations. 2012 , 116, 3021-30		67
1671	1.21 Computation of Structure, Dynamics, and Thermodynamics of Proteins. 2012 , 494-513		1
1670	Coarse-grained molecular dynamics simulations of the phase behavior of the 4-cyano-4'-pentylbiphenyl liquid crystal system. 2012 , 116, 2075-89		28
1669	Optimal number of coarse-grained sites in different components of large biomolecular complexes. 2012 , 116, 8363-74		47
1668	Assessing the relative stability of dimer interfaces in G protein-coupled receptors. 2012 , 8, e1002649		81
1667	Hybrid molecular mechanics/coarse-grained simulations for structural prediction of G-protein coupled receptor/ligand complexes. 2012 , 7, e47332		38
1666	Practical Estimation of TCR-pMHC Binding Free-Energy Based on the Dielectric Model and the Coarse-Grained Model. 2012 ,		
1665	A Review of Physics-Based Coarse-Grained Potentials for the Simulations of Protein Structure and Dynamics. 2012 , 8, 129-148		18
1664	The role of domain: domain interactions versus domain: water interactions in the coarse-grained simulations of the E1P to E2P transitions in Ca-ATPase (SERCA). 2012 , 80, 1929-47		12
1663	Coarse grain lipid-protein molecular interactions and diffusion with MsbA flippase. 2012 , 80, 2178-90		21
1662	A novel computer simulation method for simulating the multiscale transduction dynamics of signal proteins. 2012 , 136, 124112		12
1661	Modeling the Self-Assembly and Stability of DHPC Micelles Using Atomic Resolution and Coarse Grained MD Simulations. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1556-69	6.4	28
1660	Improving Internal Peptide Dynamics in the Coarse-Grained MARTINI Model: Toward Large-Scale Simulations of Amyloid- and Elastin-like Peptides. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1774-1785	6.4	63
1659	On Atomistic and Coarse-Grained Models for C60 Fullerene. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1370-8	6.4	107
1658	Biomolecular simulation: a computational microscope for molecular biology. 2012 , 41, 429-52		746
1657	Organization, dynamics, and segregation of Ras nanoclusters in membrane domains. 2012 , 109, 8097-102		130
1656	Secondary Structure Analysis of Native Cellulose by Molecular Dynamics Simulations with Coarse Grained Model. 2012 , 25, 191-198		7
1655	Bendix: intuitive helix geometry analysis and abstraction. 2012 , 28, 2193-4		87

1654	A coarse-grained model for β -d-glucose based on force matching. 2012 , 131, 1		10
1653	Structural modelling and dynamics of proteins for insights into drug interactions. 2012 , 64, 323-43		24
1652	Rapid flip-flop motions of diacylglycerol and ceramide in phospholipid bilayers. 2012 , 522, 96-102		39
1651	How SNARE molecules mediate membrane fusion: recent insights from molecular simulations. 2012 , 22, 187-96		109
1650	Coarse-grained molecular simulations of large biomolecules. 2012 , 22, 130-7		180
1649	Computer simulation studies of self-assembling macromolecules. 2012 , 22, 175-86		95
1648	Molecular dynamics simulation of hydrated DPPC monolayers using charge equilibration force fields. 2012 , 33, 141-52		15
1647	Thermodynamics and kinetics of large-time-step molecular dynamics. 2012 , 33, 475-83		10
1646	Hybrid particle-field molecular dynamics simulations: parallelization and benchmarks. 2012 , 33, 868-80		52
1645	Multiscale simulation of small peptides: consistent conformational sampling in atomistic and coarse-grained models. 2012 , 33, 937-49		21
1644	A molecular dynamics simulation study of nanomechanical properties of asymmetric lipid bilayer. 2013 , 246, 67-73		1
1643	Electronic properties of a graphene device with peptide adsorption: insight from simulation. 2013 , 5, 7470-7		56
1642	Lipid-Protein Interactions. 2013 ,		20
1641	Perspective on the Martini model. 2013 , 42, 6801-22		805
1640	Toward optimized potential functions for protein-protein interactions in aqueous solutions: osmotic second virial coefficient calculations using the MARTINI coarse-grained force field. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9,	6.4	84
1639	Electrostatic-Consistent Coarse-Grained Potentials for Molecular Simulations of Proteins. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 3515-26	6.4	27
1638	Simple Method for Simulating the Mixture of Atomistic and Coarse-Grained Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 3728-39	6.4	26
1637	Computer simulation of lipid membranes: Methodology and achievements. 2013 , 55, 162-180		22

1636	Coarse grained molecular dynamics of engineered macromolecules for the inhibition of oxidized low-density lipoprotein uptake by macrophage scavenger receptors. 2013 , 14, 2499-509	7
1635	Nanofiber-based delivery of therapeutic peptides to the brain. 2013 , 7, 1016-26	60
1634	Drug Delivery Systems: Advanced Technologies Potentially Applicable in Personalised Treatment. 2013 ,	6
1633	Atomistic and Coarse-Grained Molecular Dynamics Simulations of Membrane Proteins. 2013 , 193-206	1
1632	Study of Proteins and Peptides at Interfaces by Molecular Dynamics Simulation Techniques. 2013 , 291-313	1
1631	Exo70 generates membrane curvature for morphogenesis and cell migration. 2013 , 26, 266-78	78
1630	Materiomics: Multiscale Mechanics of Biological Materials and Structures. 2013 ,	10
1629	Self-assembly of amphiphilic peptide (AF)6H5K15: coarse-grained molecular dynamics simulation. 2013 , 117, 9690-8	31
1628	Perspective: Coarse-grained models for biomolecular systems. 2013 , 139, 090901	532
1627	Interactions of the auxilin-1 PTEN-like domain with model membranes result in nanoclustering of phosphatidyl inositol phosphates. 2013 , 105, 137-45	22
1626	Computational investigations of a Peptide-modified dendrimer interacting with lipid membranes. 2013 , 34, 1237-42	24
1625	Interfacial properties of high-density lipoprotein-like lipid droplets with different lipid and apolipoprotein A-I compositions. 2013 , 104, 2193-201	10
1624	In vivo trp scanning of the small multidrug resistance protein EmrE confirms 3D structure models'. 2013 , 425, 4642-51	14
1623	Effects of ATP and actin-filament binding on the dynamics of the myosin II S1 domain. 2013 , 105, 1624-34	12
1622	From Multiscale Modeling to Meso-Science. 2013 ,	44
1621	Membrane driven spatial organization of GPCRs. 2013 , 3, 2909	86
1620	Characterization of a membrane-active peptide from the Bordetella pertussis CyaA toxin. 2013 , 288, 32585-32598	36
1619	Computational methods of studying the binding of toxins from venomous animals to biological ion channels: theory and applications. 2013 , 93, 767-802	42

1618	Cell membranes open "doors" for cationic nanoparticles/biomolecules: insights into uptake kinetics. 2013 , 7, 10799-808		194
1617	Physicochemical properties of nanoparticles regulate translocation across pulmonary surfactant monolayer and formation of lipoprotein corona. 2013 , 7, 10525-33		142
1616	Coarse-Grained Models for Protein-Cell Membrane Interactions. 2013 , 5, 890-936		39
1615	Engineering antimicrobial peptides with improved antimicrobial and hemolytic activities. 2013 , 53, 3280-96		66
1614	An atomistic model for assembly of transmembrane domain of T cell receptor complex. 2013 , 135, 2188-97		15
1613	Branched oligopeptides form nanocapsules with lipid vesicle characteristics. 2013 , 29, 14648-54		20
1612	Effects of PEGylation on the binding interaction of magainin 2 and tachyplesin I with lipid bilayer surface. 2013 , 29, 14214-21		24
1611	MCMC2 : A Monte Carlo code for multiply-charged clusters. 2013 , 184, 873-884		7
1610	Conformational flexibility of the leucine binding protein examined by protein domain coarse-grained molecular dynamics. 2013 , 19, 4931-45		14
1609	Why do arginine and lysine organize lipids differently? Insights from coarse-grained and atomistic simulations. 2013 , 117, 12145-56		52
1608	PRIMO: A Transferable Coarse-grained Force Field for Proteins. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 3769-3788	6.4	71
1607	Coarse-Grained Potentials for Local Interactions in Unfolded Proteins. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 432-40	6.4	39
1606	Identification of cardiolipin binding sites on cytochrome c oxidase at the entrance of proton channels. 2013 , 3, 1263		112
1605	Interaction of pristine and functionalized carbon nanotubes with lipid membranes. 2013 , 117, 12113-23		51
1604	Numerical study on thermal conductivity of nanomaterials - coarse Grained Molecular Dynamics Approach. 2013 ,		0
1603	MuSTAR MD: multi-scale sampling using temperature accelerated and replica exchange molecular dynamics. 2013 , 139, 145105		24
1602	Coarse grained molecular dynamics study of heat transfer in thermal interface materials. 2013 ,		0
1601	The structural basis of ZMPSTE24-dependent laminopathies. 2013 , 339, 1604-7		75

1600	Critical cross-linking to mechanically couple polyelectrolytes and flexible molecules. 2013 , 9, 1076-1090		10
1599	Sequence dependent lipid-mediated effects modulate the dimerization of ErbB2 and its associative mutants. 2013 , 15, 19031-41		17
1598	Lipid mediated packing of transmembrane helices in a dissipative particle dynamics study. 2013 , 9, 2673		14
1597	The Martini coarse-grained force field. 2013 , 924, 533-65		79
1596	Computer simulation studies of counterion effects on the properties of surfactant systems. 2013 , 18, 15-25		31
1595	Effect of sodium chloride on the structure and stability of spider silk's N-terminal protein domain. 2013 , 1, 276-284		29
1594	Simulation-based prediction of phosphatidylinositol 4,5-bisphosphate binding to an ion channel. 2013 , 52, 279-81		54
1593	Theoretical and computational studies of dendrimers as delivery vectors. 2013 , 42, 705-27		175
1592	Improved Parameters for the Martini Coarse-Grained Protein Force Field. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 687-97	6.4	782
1591	Multiscale molecular dynamics simulations of membrane proteins. 2013 , 924, 635-57		16
1590	Anomalous and normal diffusion of proteins and lipids in crowded lipid membranes. 2013 , 161, 397-417; discussion 419-59		146
1589	Dodecyl maltoside protects membrane proteins in vacuo. 2013 , 105, 648-56		19
1588	In silico design of anti-atherogenic biomaterials. 2013 , 34, 7950-9		16
1587	Computational Studies of Biomembrane Systems: Theoretical Considerations, Simulation Models, and Applications. 2013 , 237-283		13
1586	Free energy profile and mechanism of self-assembly of peptide amphiphiles based on a collective assembly coordinate. 2013 , 117, 9004-13		22
1585	Free-energy landscape for peptide amphiphile self-assembly: stepwise versus continuous assembly mechanisms. 2013 , 117, 14059-64		21
1584	Generation and sensing of membrane curvature: Where materials science and biophysics meet. 2013 , 17, 164-174		19
1583	Bacteriocin AS-48 binding to model membranes and pore formation as revealed by coarse-grained simulations. 2013 , 1828, 2524-31		28

1582	Structural determinants of specific lipid binding to potassium channels. 2013 , 135, 3983-8	65
1581	Carbon nanotube bundling: influence on layer-by-layer assembly and antimicrobial activity. 2013 , 9, 2136	26
1580	Mixing MARTINI: electrostatic coupling in hybrid atomistic-coarse-grained biomolecular simulations. 2013 , 117, 3516-30	117
1579	Free energy of WALP23 dimer association in DMPC, DPPC, and DOPC bilayers. 2013 , 169, 95-105	92
1578	Nanomechanical properties of lipid bilayer: asymmetric modulation of lateral pressure and surface tension due to protein insertion in one leaflet of a bilayer. 2013 , 138, 065101	7
1577	A general method for spatially coarse-graining Metropolis Monte Carlo simulations onto a lattice. 2013 , 138, 114104	3
1576	Translocation of polyarginines and conjugated nanoparticles across asymmetric membranes. 2013 , 9, 1281-1286	59
1575	Defining the membrane-associated state of the PTEN tumor suppressor protein. 2013 , 104, 613-21	35
1574	The simulation approach to lipid-protein interactions. 2013 , 974, 435-55	3
1573	The association of polar residues in the DAP12 homodimer: TOXCAT and molecular dynamics simulation studies. 2013 , 104, 1435-44	19
1572	The Theory of Ultra-Coarse-Graining. 1. General Principles. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2466-80	6.4 114
1571	Melittin creates transient pores in a lipid bilayer: results from computer simulations. 2013 , 117, 5031-42	47
1570	Interaction of human synovial phospholipase A2 with mixed lipid bilayers: a coarse-grain and all-atom molecular dynamics simulation study. 2013 , 52, 1477-89	14
1569	Martini Force Field Parameters for Glycolipids. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 1694-708	6.4 127
1568	The addressing fragment of mitogaligin: first insights into functional and structural properties. 2013 , 14, 711-20	
1567	Dimers of human α -defensins and their interactions with the POPG membrane. 2013 , 39, 849-859	3
1566	Multiscale simulations reveal conserved patterns of lipid interactions with aquaporins. 2013 , 21, 810-9	64
1565	Multi-scale modeling of biomaterials and tissues. 2013 , 13-55	3

1564	Multiscale modeling of diffusion phenomena in polymers. 2013 , 71-86		
1563	Comparing simulations of lipid bilayers to scattering data: the GROMOS 43A1-S3 force field. 2013 , 117, 5065-72		42
1562	Systematic methods for structurally consistent coarse-grained models. 2013 , 924, 487-531		53
1561	Analytical model and multiscale simulations of α -peptide aggregation in lipid membranes: towards a unifying description of conformational transitions, oligomerization and membrane damage. 2013 , 15, 8940-51		43
1560	The shape and free energy of a lipid bilayer surrounding a membrane inclusion. 2013 , 169, 2-8		1
1559	Study on Interfacial Interaction between Polymer and Nanoparticle in a Nanocoating Matrix: A MARTINI Coarse-Graining Method. 2013 , 52, 73-82		21
1558	Homogeneous Hydrophobic-Hydrophilic Surface Patterns Enhance Permeation of Nanoparticles through Lipid Membranes. 2013 , 4, 1907-12		56
1557	Correlation of nanoscale organizations of polymer and nanocrystals in polymer/inorganic nanocrystal bulk heterojunction hybrid solar cells: insights from multiscale molecular simulations. 2013 , 6, 307-315		16
1556	Effect of arginine-rich peptide length on the structure and binding strength of siRNA-peptide complexes. 2013 , 117, 6917-26		16
1555	Improved Angle Potentials for Coarse-Grained Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 3282-92	6.4	45
1554	Solvent-Responsive Behavior of Polymer-Brush-Modified Amphiphilic Gold Nanoparticles. 2013 , 22, 174-186		30
1553	In Silico Research in Drug Delivery Systems. 2013 , 271-313		
1552	Three-dimensional stress field around a membrane protein: atomistic and coarse-grained simulation analysis of gramicidin A. 2013 , 104, 117-27		24
1551	Dynamic Heterogeneity in Random and Gradient Copolymers: A Computational Investigation. 2013 , 46, 5066-5079		26
1550	A molecular dynamics simulation of N-(fluorenyl-9-methoxycarbonyl)-dipeptides supramolecular hydrogel. 2013 , 417, 217-223		14
1549	Molecular-Cluster-Assembly Method for Analysis of High-Dimensional Structures of p-Cresol Chains in Phenolic Polymers. 2013 , 22, 443-461		2
1548	PaLaCe: A Coarse-Grain Protein Model for Studying Mechanical Properties. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 785-93	6.4	37
1547	A hybrid particle-field molecular dynamics approach: a route toward efficient coarse-grained models for biomembranes. 2013 , 10, 045007		23

1546	Deformation of a Two-domain Lipid Bilayer due to Asymmetric Insertion of Lipid-modified Ras Peptides. 2013 , 9,		16
1545	Structure-based coarse-graining for inhomogeneous liquid polymer systems. 2013 , 139, 054901		12
1544	Modeling Protein-Protein Recognition in Solution Using the Coarse-Grained Force Field SCORPION. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 803-13	6.4	33
1543	MD simulations suggest important surface differences between reconstituted and circulating spherical HDL. 2013 , 54, 2718-32		12
1542	Insight into β -synuclein plasticity and misfolding from differential micelle binding. 2013 , 117, 11448-59		11
1541	A Charge Moving Algorithm for Molecular Dynamics Simulations of Gas-Phase Proteins. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2531-9	6.4	35
1540	Synthesize multiblock copolymers via complex formations between β -cyclodextrin and adamantane groups terminated at diblock copolymer ends: a Brownian dynamics simulation study. 2013 , 117, 16283-91		5
1539	Evidence for cardiolipin binding sites on the membrane-exposed surface of the cytochrome bc1. 2013 , 135, 3112-20		126
1538	Surface-Tension Replica-Exchange Molecular Dynamics Method for Enhanced Sampling of Biological Membrane Systems. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 5629-40	6.4	33
1537	Effects of flanking loops on membrane insertion of transmembrane helices: a role for peptide conformational equilibrium. 2013 , 117, 8330-9		4
1536	Combining coarse-grained nonbonded and atomistic bonded interactions for protein modeling. 2013 , 81, 81-92		21
1535	Molecular view on protein sorting into liquid-ordered membrane domains mediated by gangliosides and lipid anchors. 2013 , 161, 347-63; discussion 419-59		63
1534	Coarse-grained models for protein folding and aggregation. 2013 , 924, 585-600		6
1533	Dynamics of discrete semiflexible chains under dihedral constraints: analytic results. 2013 , 138, 204902		6
1532	SAHBNET, an accessible surface-based elastic network: an application to membrane protein. 2013 , 14, 11510-26		8
1531	Reduced lateral mobility of lipids and proteins in crowded membranes. 2013 , 9, e1003033		120
1530	Formation of raft-like assemblies within clusters of influenza hemagglutinin observed by MD simulations. 2013 , 9, e1003034		43
1529	Insertion of the Ca^{2+} -independent phospholipase A ₂ into a phospholipid bilayer via coarse-grained and atomistic molecular dynamics simulations. 2013 , 9, e1003156		27

1528	Conformational changes in talin on binding to anionic phospholipid membranes facilitate signaling by integrin transmembrane helices. 2013 , 9, e1003316	23
1527	Exploring amyloid aggregates with coarse-grained protein simulations. 2013 , 1535, 6001	
1526	Intracellular trafficking of the KV1.3 potassium channel is regulated by the prodomain of a matrix metalloprotease. 2013 , 288, 6451-64	16
1525	Molecular modeling of protein materials: case study of elastin. 2013 , 21, 063001	9
1524	Helical structures drive early stages of self-assembly of amyloidogenic amyloid polypeptide aggregate formation in membranes. 2013 , 3, 2781	79
1523	Toward Structure Prediction for Short Peptides Using the Improved SAAP Force Field Parameters. 2013 , 2013, 1-13	3
1522	The role of electrostatics and temperature on morphological transitions of hydrogel nanostructures self-assembled by peptide amphiphiles via molecular dynamics simulations. 2013 , 2, 1388-400	38
1521	Nonlinear intrinsic variables and state reconstruction in multiscale simulations. 2013 , 139, 184109	19
1520	Modelling and computer simulation of food structures. 2013 , 336-385	4
1519	Role of the C-terminal domain in the structure and function of tetrameric sodium channels. 2013 , 4, 2465	59
1518	Thermodynamic analysis of structural transitions during GNNQQNY aggregation. 2013 , 81, 1141-55	20
1517	Nanomechanics of collagen microfibrils. 2013 , 3, 23-34	18
1516	Validating a Coarse-Grained Potential Energy Function through Protein Loop Modelling. 2013 , 8, e65770	12
1515	Optimization of an elastic network augmented coarse grained model to study CCMV capsid deformation. 2013 , 8, e60582	35
1514	Stability of transmembrane amyloid β -peptide and membrane integrity tested by molecular modeling of site-specific A β 42 mutations. 2013 , 8, e78399	26
1513	Molecular basis for the dissociation dynamics of protein A-immunoglobulin G1 complex. 2013 , 8, e66935	7
1512	Cholesterol induces uneven curvature of asymmetric lipid bilayers. 2013 , 2013, 965230	32
1511	Molecular mechanics and dynamics: numerical tools to sample the configuration space. 2014 , 19, 578-604	11

1510	Atomic resolution view into the structure-function relationships of the human myelin peripheral membrane protein P2. 2014 , 70, 165-76	31
1509	Differential stability of the crystallographic interfaces of mu- and kappa-opioid receptors. 2014 , 9, e90694	22
1508	Transmembrane recognition of the semaphorin co-receptors neuropilin 1 and plexin A1: coarse-grained simulations. 2014 , 9, e97779	20
1507	Dynamic scenario of membrane binding process of kalata b1. 2014 , 9, e114473	6
1506	Complex Molecules at Liquid Interfaces: Insights from Molecular Simulation. 2014 , 2014, 1-12	8
1505	Molecular Modeling to Study Dendrimers for Biomedical Applications. 2014 , 19, 20424-20467	52
1504	Complementary Co-assembling Peptides: From In Silico Studies to In Vivo Application. 2014 , 24, 6317-6328	34
1503	Beyond standard molecular dynamics: investigating the molecular mechanisms of G protein-coupled receptors with enhanced molecular dynamics methods. 2014 , 796, 95-125	14
1502	Molecular Dynamics Simulations of Competitive Protein Adsorption onto Chromatographic Media. 2014 , 33, 937-942	
1501	The X-ray structure of NccX from <i>Cupriavidus metallidurans</i> 31A illustrates potential dangers of detergent solubilization when generating and interpreting crystal structures of membrane proteins. 2014 , 289, 31160-72	9
1500	The influence of fatty acids on the GpA dimer interface by coarse-grained molecular dynamics simulation. 2014 , 15, 14247-68	2
1499	Lipid clustering correlates with membrane curvature as revealed by molecular simulations of complex lipid bilayers. 2014 , 10, e1003911	160
1498	The free energy landscape of dimerization of a membrane protein, NanC. 2014 , 10, e1003417	23
1497	A multiscale approach to modelling drug metabolism by membrane-bound cytochrome P450 enzymes. 2014 , 10, e1003714	38
1496	Hydrophobic compounds reshape membrane domains. 2014 , 10, e1003873	42
1495	Interactions of borneol with DPPC phospholipid membranes: a molecular dynamics simulation study. 2014 , 15, 20365-81	11
1494	Assembly of Nsp1 nucleoporins provides insight into nuclear pore complex gating. 2014 , 10, e1003488	36
1493	NRas slows the rate at which a model lipid bilayer phase separates. 2014 , 169, 209-23	16

1492	Modeling Non-Native Interactions in Designed Proteins. 2014 , 54, 1230-1240	16
1491	Effect of hydrophobic mismatch on domain formation and peptide sorting in the multicomponent lipid bilayers in the presence of immobilized peptides. 2014 , 141, 074702	12
1490	Fluctuating hydrodynamics of multicomponent membranes with embedded proteins. 2014 , 141, 075103	21
1489	Reconciling structural and thermodynamic predictions using all-atom and coarse-grain force fields: the case of charged oligo-arginine translocation into DMPC bilayers. 2014 , 118, 11973-92	12
1488	New strategies for integrative dynamic modeling of macromolecular assembly. 2014 , 96, 77-111	8
1487	Reactive molecular dynamics study of the pH-dependent dynamic structure of β helix. 2014 , 118, 13498-504	6
1486	Modeling the effect of nano-sized polymer particles on the properties of lipid membranes. 2014 , 26, 503101	25
1485	The Treatment of Solvent in Multiscale Biophysical Modeling. 2014 , 54, 1074-1083	8
1484	More than the sum of its parts: coarse-grained peptide-lipid interactions from a simple cross-parametrization. 2014 , 140, 115101	33
1483	Membrane remodeling capacity of a vesicle-inducing glycosyltransferase. 2014 , 281, 3667-84	16
1482	Recent advances in transferable coarse-grained modeling of proteins. 2014 , 96, 143-80	33
1481	Mathematical and computational modeling in biology at multiple scales. 2014 , 11, 52	7
1480	Molecular dynamics simulation of membrane proteins. 2014 , 805, 305-29	10
1479	Computer Simulations of Soft Matter: Linking the Scales. 2014 , 16, 4199-4245	73
1478	Functional truncated membrane pores. 2014 , 111, 2425-30	53
1477	A conformational landscape for alginate secretion across the outer membrane of <i>Pseudomonas aeruginosa</i> . 2014 , 70, 2054-68	37
1476	Simulations suggest possible novel membrane pore structure. 2014 , 30, 1304-10	17
1475	Modelling and enhanced molecular dynamics to steer structure-based drug discovery. 2014 , 114, 123-36	29

1474	Modeling of Membrane Proteins. 2014 , 357-431		
1473	The power of coarse graining in biomolecular simulations. 2014 , 4, 225-248		346
1472	Protein Conformational Dynamics. 2014 ,		9
1471	Controlling dissociation channels of gas-phase protein complexes using charge manipulation. 2014 , 25, 722-8		6
1470	Theoretical considerations and computational tools. 2014 , 794, 69-93		
1469	Cholesterol modulates the dimer interface of the β adrenergic receptor via cholesterol occupancy sites. 2014 , 106, 1290-300		122
1468	Plasticity and conformational equilibria of influenza fusion peptides in model lipid bilayers. 2014 , 1838, 1169-79		9
1467	Dynamics and stability of lipid bilayers modulated by thermosensitive polypeptides, cholesterol, and PEGylated lipids. 2014 , 16, 3763-70		13
1466	A global machine learning based scoring function for protein structure prediction. 2014 , 82, 752-9		20
1465	Live-cell imaging of phosphatidic acid dynamics in pollen tubes visualized by Spo20p-derived biosensor. 2014 , 203, 483-494		58
1464	Molecular Dynamics Studies of Liposomes as Carriers for Photosensitizing Drugs: Development, Validation, and Simulations with a Coarse-Grained Model. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5-13	6.4	31
1463	Mechanism of activation of protein kinase JAK2 by the growth hormone receptor. 2014 , 344, 1249783		269
1462	Transport and dielectric properties of water and the influence of coarse-graining: comparing BMW, SPC/E, and TIP3P models. 2014 , 140, 064107		45
1461	Simulations of Protein Aggregation: Insights from Atomistic and Coarse-Grained Models. 2014 , 5, 1899-908		76
1460	Size-Selective, Noncovalent Dispersion of Carbon Nanotubes by PEGylated Lipids: A Coarse-Grained Molecular Dynamics Study. 2014 , 59, 3080-3089		18
1459	Aqueous poly(amidoamine) dendrimer G3 and G4 generations with several interior cores at pHs 5 and 7: a molecular dynamics simulation study. 2014 , 118, 3257-66		21
1458	Delaunay-based nonlocal interactions are sufficient and accurate in protein fold recognition. 2014 , 82, 415-23		7
1457	G Protein-Coupled Receptors - Modeling and Simulation. 2014 ,		7

1456	Multiscale modelling to understand the self-assembly mechanism of human β_2 -adrenergic receptor in lipid bilayer. 2014 , 48, 29-39		26
1455	Computer simulation techniques for food science and engineering: Simulating atomic scale and coarse-grained models. 2014 , 1, 71-90		6
1454	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
1453	Coarse-grained versus atomistic simulations: realistic interaction free energies for real proteins. 2014 , 30, 326-34		28
1452	Transmembrane fragment structures of amyloid precursor protein depend on membrane surface curvature. 2014 , 136, 854-7		44
1451	Primary and secondary dimer interfaces of the fibroblast growth factor receptor 3 transmembrane domain: characterization via multiscale molecular dynamics simulations. 2014 , 53, 323-32		20
1450	A Systems Biology Approach to Study Metabolic Syndrome. 2014 ,		1
1449	Multiscale computational models in physical systems biology of intracellular trafficking. 2014 , 8, 198-213		19
1448	How does growth hormone releasing hexapeptide self-assemble in nanotubes?. 2014 , 10, 9260-9		5
1447	Potential of mean force analysis of the self-association of leucine-rich transmembrane β -helices: difference between atomistic and coarse-grained simulations. 2014 , 141, 075101		11
1446	A coarse-graining approach for molecular simulation that retains the dynamics of the all-atom reference system by implementing hydrodynamic interactions. 2014 , 141, 174107		18
1445	Free energy landscape of rim-pore expansion in membrane fusion. 2014 , 107, 2287-95		20
1444	Local pressure changes in lipid bilayers due to adsorption of melittin and magainin-h2 antimicrobial peptides: results from computer simulations. 2014 , 118, 12673-9		10
1443	Cholesterol, sphingolipids, and glycolipids: what do we know about their role in raft-like membranes?. 2014 , 184, 82-104		133
1442	Tunable Coarse Graining for Monte Carlo Simulations of Proteins via Smoothed Energy Tables: Direct and Exchange Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5161-5177	6.4	7
1441	The OPEP protein model: from single molecules, amyloid formation, crowding and hydrodynamics to DNA/RNA systems. 2014 , 43, 4871-93		118
1440	Surface tension effects on the phase transition of a DPPC bilayer with and without protein: a molecular dynamics simulation. 2014 , 16, 8434-40		8
1439	Thermodynamics of antimicrobial lipopeptide binding to membranes: origins of affinity and selectivity. 2014 , 107, 1862-1872		25

1438	Mesoscale computational studies of membrane bilayer remodeling by curvature-inducing proteins. 2014 , 543, 1-60		44
1437	Coarse-graining poly(ethylene oxide)-poly(propylene oxide)-poly(ethylene oxide) (PEO-PPO-PEO) block copolymers using the MARTINI force field. 2014 , 118, 1648-59		52
1436	Improved Coarse-Grained Modeling of Cholesterol-Containing Lipid Bilayers. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2137-2150	6.4	31
1435	Interactions of peripheral proteins with model membranes as viewed by molecular dynamics simulations. 2014 , 42, 1418-24		29
1434	Methodologies for the analysis of instantaneous lipid diffusion in MD simulations of large membrane systems. 2014 , 169, 455-75		27
1433	Multi-scale modeling of mycosubtilin lipopeptides at the air/water interface: structure and optical second harmonic generation. 2014 , 16, 2136-48		6
1432	Coarse-grained modeling of peptidic/PDMS triblock morphology. 2014 , 118, 13718-28		9
1431	Global structural changes of an ion channel during its gating are followed by ion mobility mass spectrometry. 2014 , 111, 17170-5		54
1430	Promote potential applications of nanoparticles as respiratory drug carrier: insights from molecular dynamics simulations. 2014 , 6, 2759-67		51
1429	COFFDROP: A Coarse-Grained Nonbonded Force Field for Proteins Derived from All-Atom Explicit-Solvent Molecular Dynamics Simulations of Amino Acids. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5178-5194	6.4	12
1428	Lipid structure in triolein lipid droplets. 2014 , 118, 10335-40		17
1427	Lipid organization of the plasma membrane. 2014 , 136, 14554-9		519
1426	Construction of an intermediate-resolution lattice model and re-examination of the helix-coil transition: a dynamic Monte Carlo simulation. 2014 , 32, 792-803		1
1425	Role of hydrophobicity on self-assembly by peptide amphiphiles via molecular dynamics simulations. 2014 , 30, 7745-54		45
1424	Polystyrene Nanoparticles Perturb Lipid Membranes. 2014 , 5, 241-6		174
1423	Free Energy Calculations for the Peripheral Binding of Proteins/Peptides to an Anionic Membrane. 1. Implicit Membrane Models. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2845-59	6.4	19
1422	Oleic acid phase behavior from molecular dynamics simulations. 2014 , 30, 10661-7		46
1421	Understanding selective molecular recognition in integrated carbon nanotube-polymer sensors by simulating physical analyte binding on carbon nanotube-polymer scaffolds. 2014 , 10, 5991-6004		8

1420	Sidekick for Membrane Simulations: Automated Ensemble Molecular Dynamics Simulations of Transmembrane Helices. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2165-75	6.4	22
1419	Interactions of phosphatase and tensin homologue (PTEN) proteins with phosphatidylinositol phosphates: insights from molecular dynamics simulations of PTEN and voltage sensitive phosphatase. 2014 , 53, 1724-32		35
1418	Assembly of amyloid β peptides in the presence of fibril seeds: one-pot coarse-grained molecular dynamics simulations. 2014 , 118, 9238-46		16
1417	Molecular dynamics studies of PEGylated β helical coiled coils and their self-assembled micelles. 2014 , 30, 8848-55		16
1416	Self-assembly of amphiphilic peptide (AF)6H5K15 derivatives: roles of hydrophilic and hydrophobic residues. 2014 , 118, 2683-92		18
1415	Perspectives on the simulation of protein-surface interactions using empirical force field methods. 2014 , 124, 25-37		36
1414	Interplay between curvature and lateral organization of lipids and peptides/proteins in model membranes. 2014 , 30, 1116-22		21
1413	An Anisotropic Coarse-Grained Model for Proteins Based On Gay-Berne and Electric Multipole Potentials. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 731-750	6.4	30
1412	Transferability of coarse-grained force field for nCB liquid crystal systems. 2014 , 118, 4647-60		20
1411	Transferring the PRIMO Coarse-Grained Force Field to the Membrane Environment: Simulations of Membrane Proteins and Helix-Helix Association. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3459-3472	6.4	26
1410	A theoretical view of protein dynamics. 2014 , 43, 5051-66		83
1409	Atomistic models of general anesthetics for use in in silico biological studies. 2014 , 118, 12075-86		24
1408	Acceleration of Lateral Equilibration in Mixed Lipid Bilayers Using Replica Exchange with Solute Tempering. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4264-4272	6.4	32
1407	Determining Structural and Mechanical Properties from Molecular Dynamics Simulations of Lipid Vesicles. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4160-4168	6.4	19
1406	The importance of membrane defects-lessons from simulations. 2014 , 47, 2244-51		59
1405	Role of Backbone Dipole Interactions in the Formation of Secondary and Supersecondary Structures of Proteins. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2569-2576	6.4	21
1404	CHARMM-GUI PACE CG Builder for solution, micelle, and bilayer coarse-grained simulations. 2014 , 54, 1003-9		33
1403	A unified coarse-grained model of biological macromolecules based on mean-field multipole-multipole interactions. 2014 , 20, 2306		83

1402	Dimerization of the EphA1 receptor tyrosine kinase transmembrane domain: Insights into the mechanism of receptor activation. 2014 , 53, 6641-52	32
1401	Does the Like Dissolves Like Rule Hold for Fullerene and Ionic Liquids?. 2014 , 43, 1019-1031	37
1400	Coarse-Graining of TIP4P/2005, TIP4P-Ew, SPC/E, and TIP3P to Monatomic Anisotropic Water Models Using Relative Entropy Minimization. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4104-20	6.4 86
1399	De novo inference of protein function from coarse-grained dynamics. 2014 , 82, 2443-54	8
1398	Mesoscopic coarse-grained simulations of lysozyme adsorption. 2014 , 118, 4451-60	52
1397	PEGylated, NH ₂ -terminated PAMAM dendrimers: a microscopic view from atomistic computer simulations. 2014 , 11, 1459-70	19
1396	Determination of mean and Gaussian curvatures of highly curved asymmetric lipid bilayers: the case study of the influence of cholesterol on the membrane shape. 2014 , 16, 17052-61	18
1395	Exploring the dynamics and interaction of a full ErbB2 receptor and Trastuzumab-Fab antibody in a lipid bilayer model using Martini coarse-grained force field. 2014 , 28, 1093-107	5
1394	Translocation thermodynamics of linear and cyclic nonaarginine into model DPPC bilayer via coarse-grained molecular dynamics simulation: implications of pore formation and nonadditivity. 2014 , 118, 2670-82	26
1393	Complementary biophysical tools to investigate lipid specificity in the interaction between bioactive molecules and the plasma membrane: A review. 2014 , 1838, 3171-3190	109
1392	Triphenylalanine peptides self-assemble into nanospheres and nanorods that are different from the nanovesicles and nanotubes formed by diphenylalanine peptides. 2014 , 6, 2800-11	83
1391	Coarse-grained molecular dynamics simulations of protein-ligand binding. 2014 , 35, 1835-45	22
1390	The activation mode of the mechanosensitive ion channel, MscL, by lysophosphatidylcholine differs from tension-induced gating. 2014 , 28, 4292-302	36
1389	Structural characterization of heparin-induced glyceraldehyde-3-phosphate dehydrogenase protofibrils preventing β -synuclein oligomeric species toxicity. 2014 , 289, 13838-50	26
1388	Ebolavirus entry requires a compact hydrophobic fist at the tip of the fusion loop. 2014 , 88, 6636-49	33
1387	Adaptive Resolution Simulation of MARTINI Solvents. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2591-8	6.4 39
1386	Resolution-Adapted All-Atomic and Coarse-Grained Model for Biomolecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2528-36	6.4 18
1385	Systematic Method for Thermomechanically Consistent Coarse-Graining: A Universal Model for Methacrylate-Based Polymers. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2514-27	6.4 82

1384	Universal Method for Embedding Proteins into Complex Lipid Bilayers for Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2577-82	6.4	31
1383	Protein and lipid interactions driving molecular mechanisms of in meso crystallization. 2014 , 136, 3271-84		15
1382	Structural heterogeneity in transmembrane amyloid precursor protein homodimer is a consequence of environmental selection. 2014 , 136, 9619-26		31
1381	Partitioning of amino acids into a model membrane: capturing the interface. 2014 , 118, 1481-92		43
1380	From Single Molecules to Nanoscopically Structured Materials. 2014 ,		3
1379	Not just an oil slick: how the energetics of protein-membrane interactions impacts the function and organization of transmembrane proteins. 2014 , 106, 2305-16		46
1378	Design and application of implicit solvent models in biomolecular simulations. 2014 , 25, 126-34		102
1377	3D hydrophobic moment vectors as a tool to characterize the surface polarity of amphiphilic peptides. 2014 , 106, 2385-94		50
1376	Computing 1-D atomic densities in macromolecular simulations: The density profile tool for VMD. 2014 , 185, 317-322		81
1375	Nonlamellar Lipid Aggregates. 2014 , 48-65		1
1374	Surface Structure and Interaction of Surface/Interface Probed by Mesoscale Simulations and Experiments. 2015 , 47, 85-162		1
1373	Defining the membrane disruption mechanism of kalata B1 via coarse-grained molecular dynamics simulations. 2014 , 4, 3933		24
1372	Strong influence of periodic boundary conditions on lateral diffusion in lipid bilayer membranes. 2015 , 143, 243113		55
1371	Folding and insertion thermodynamics of the transmembrane WALP peptide. 2015 , 143, 243127		29
1370	Hydrophobic mismatch demonstrated for membranolytic peptides, and their use as molecular rulers to measure bilayer thickness in native cells. 2015 , 5, 9388		41
1369	Coarse-grained simulations of polyelectrolyte complexes: MARTINI models for poly(styrene sulfonate) and poly(diallyldimethylammonium). 2015 , 143, 243151		55
1368	Calculating the free energy of transfer of small solutes into a model lipid membrane: Comparison between metadynamics and umbrella sampling. 2015 , 143, 144108		45
1367	Tabulation as a high-resolution alternative to coarse-graining protein interactions: Initial application to virus capsid subunits. 2015 , 143, 243159		6

1366	Transient Hairpin formation in Synuclein monomer revealed by coarse-grained molecular dynamics simulation. 2015 , 143, 243142	49
1365	On the application of the MARTINI coarse-grained model to immersion of a protein in a phospholipid bilayer. 2015 , 143, 243139	15
1364	Free-energy coarse-grained potential for C60. 2015 , 143, 164509	2
1363	Ion-Exchange Adsorption of Proteins: Experiments and Molecular Dynamics Simulations. 2015 , 87, 903-909	1
1362	Computational Investigations of Arginine-Rich Peptides Interacting with Lipid Membranes. 2015 , 24, 399-406	14
1361	Extension of a protein docking algorithm to membranes and applications to amyloid precursor protein dimerization. 2015 , 83, 2170-85	11
1360	Molecular Dynamics Simulations of Retrograde Condensation in Nanoporous Shale. 2015 ,	0
1359	Mesoscopic coarse-grained simulations of hydrophobic charge induction chromatography (HCIC) for protein purification. 2015 , 61, 2035-2047	28
1358	Computational Approaches to Understanding the Self-assembly of Peptide-based Nanostructures. 2015 , 55, 724-734	21
1357	Design of Aggregate Structures and Molecular Capture by Using Molecular-Cluster-Assembly Method. 2015 , 24, 595-609	
1356	A multiscale approach to simulating the conformational properties of unbound multi-C ₂ H ₂ Zinc finger proteins. 2015 , 83, 1604-15	1
1355	Computational Amphiphilic Materials for Drug Delivery. 2015 , 2,	17
1354	Mechanisms of recognition and binding of HTP to the plasma membrane by multi-scale molecular dynamics simulations. 2015 , 2, 36	8
1353	Assembly of Influenza Hemagglutinin Fusion Peptides in a Phospholipid Bilayer by Coarse-grained Computer Simulations. 2015 , 2, 66	6
1352	TatBC-independent TatA/Tat substrate interactions contribute to transport efficiency. 2015 , 10, e0119761	15
1351	Mapping the Protein Fold Universe Using the CamTube Force Field in Molecular Dynamics Simulations. 2015 , 11, e1004435	14
1350	A Coarse Grained Model for a Lipid Membrane with Physiological Composition and Leaflet Asymmetry. 2015 , 10, e0144814	38
1349	Molecular simulation studies of human coagulation factor VIII C domain-mediated membrane binding. 2015 , 113, 373-84	9

1348	Systematic methods for defining coarse-grained maps in large biomolecules. 2015 , 827, 33-48	6
1347	Structure and Dynamics of Phospholipid Nanodiscs from All-Atom and Coarse-Grained Simulations. 2015 , 119, 6991-7002	30
1346	Mechanism of membrane poration by shock wave induced nanobubble collapse: a molecular dynamics study. 2015 , 119, 6225-34	48
1345	MARTINI Coarse-Grained Models of Polyethylene and Polypropylene. 2015 , 119, 8209-16	66
1344	Probing the Solution Structure of I κ B Kinase (IKK) Subunit β and Its Interaction with Kaposi Sarcoma-associated Herpes Virus Flice-interacting Protein and IKK Subunit β by EPR Spectroscopy. 2015 , 290, 16539-49	14
1343	PACSAB: Coarse-Grained Force Field for the Study of Protein-Protein Interactions and Conformational Sampling in Multiprotein Systems. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5929-38	6.4 10
1342	The role of lipids in mechanosensation. 2015 , 22, 991-8	111
1341	Dynamic Modeling of Antimicrobial Pore Formation in Engineered Tethered Membranes. 2015 , 1, 265-276	3
1340	Bicelles and Other Membrane Mimics: Comparison of Structure, Properties, and Dynamics from MD Simulations. 2015 , 119, 15831-43	31
1339	Reversible Effects of Peptide Concentration and Lipid Composition on H-Ras Lipid Anchor Clustering. 2015 , 109, 2467-2470	21
1338	Coarse-grained molecular dynamics simulation of self-assembly and surface adsorption of ionic surfactants using an implicit water model. 2015 , 31, 1262-71	57
1337	Ribonuclease A adsorption onto charged self-assembled monolayers: A multiscale simulation study. 2015 , 121, 331-339	34
1336	Multiscale approach to investigate self-assembly of telodendrimer based nanocarriers for anticancer drug delivery. 2015 , 31, 4270-80	30
1335	Surface-functionalized nanoparticle permeation triggers lipid displacement and water and ion leakage. 2015 , 31, 1074-85	28
1334	Probing structural determinants of ATP-binding cassette exporter conformational transition using coarse-grained molecular dynamics. 2015 , 119, 1295-301	12
1333	Mechanics of membrane fusion/pore formation. 2015 , 185, 109-28	35
1332	Membrane Association of the Diphtheria Toxin Translocation Domain Studied by Coarse-Grained Simulations and Experiment. 2015 , 248, 529-43	7
1331	Computational studies of protein aggregation: methods and applications. 2015 , 66, 643-66	131

1330	Solvent effects on kinetic mechanisms of self-assembly by peptide amphiphiles via molecular dynamics simulations. 2015 , 31, 315-24	42
1329	Shock Wave Induced Collapse of Arrays of Nanobubbles Located Next to a Lipid Membrane: Coarse-Grained Computer Simulations. 2015 , 119, 8879-89	20
1328	Controlling carbon-nanotube-phospholipid solubility by curvature-dependent self-assembly. 2015 , 119, 4020-32	13
1327	MARTINI coarse-grained model for crystalline cellulose microfibrils. 2015 , 119, 465-73	39
1326	Multiscale modeling of four-component lipid mixtures: domain composition, size, alignment, and properties of the phase interface. 2015 , 119, 4240-50	69
1325	Coarse-grain simulations of skin ceramide NS with newly derived parameters clarify structure of melted phase. 2015 , 119, 3988-98	20
1324	A structural mechanism for calcium transporter headpiece closure. 2015 , 119, 1407-15	20
1323	Coarse-grained model of glycosaminoglycans. 2015 , 55, 114-24	32
1322	Signaling factor interactions with polysaccharide aggregates of bacterial biofilms. 2015 , 31, 1958-66	4
1321	C ₆₀ fullerene promotes lung monolayer collapse. 2015 , 12, 20140931	29
1320	Investigating Hydrophilic Pores in Model Lipid Bilayers Using Molecular Simulations: Correlating Bilayer Properties with Pore-Formation Thermodynamics. 2015 , 31, 6615-31	34
1319	Coarse-grained simulation of cellulose I β with application to long fibrils. 2015 , 22, 31-44	23
1318	Simulating the antimicrobial mechanism of human α -defensin-3 with coarse-grained molecular dynamics. 2015 , 33, 2522-9	14
1317	Dynamics of CYP51: implications for function and inhibitor design. 2015 , 28, 59-73	27
1316	Evaluating Force Fields for the Computational Prediction of Ionized Arginine and Lysine Side-Chains Partitioning into Lipid Bilayers and Octanol. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 1775-91	30
1315	Molecular basis of endosomal-membrane association for the dengue virus envelope protein. 2015 , 1848, 1041-52	18
1314	N-Lipidated Peptide Dimers: Effective Antibacterial Agents against Gram-Negative Pathogens through Lipopolysaccharide Permeabilization. 2015 , 58, 6533-48	32
1313	Toward Improved Force-Field Accuracy through Sensitivity Analysis of Host-Guest Binding Thermodynamics. 2015 , 119, 10145-55	25

1312	Nanodomain Formation of Ganglioside GM1 in Lipid Membrane: Effects of Cholera Toxin-Mediated Cross-Linking. 2015 , 31, 9105-14		27
1311	Insights into the Packing Switching of the EphA2 Transmembrane Domain by Molecular Dynamic Simulations. 2015 , 119, 7816-24		13
1310	Nothing to sneeze at: a dynamic and integrative computational model of an influenza A virion. 2015 , 23, 584-597		71
1309	Molecular dynamics simulations of the bacterial UraA H ⁺ -uracil symporter in lipid bilayers reveal a closed state and a selective interaction with cardiolipin. 2015 , 11, e1004123		30
1308	Surface Density-Induced Pleating of a Lipid Monolayer Drives Nascent High-Density Lipoprotein Assembly. 2015 , 23, 1214-26		34
1307	Coarse-Graining the Liquid-Liquid Interfaces with the MARTINI Force Field: How Is the Interfacial Tension Reproduced?. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 3818-28	6.4	31
1306	The juxtamembrane regions of human receptor tyrosine kinases exhibit conserved interaction sites with anionic lipids. 2015 , 5, 9198		69
1305	Size controlled protein nanoemulsions for active targeting of folate receptor positive cells. 2015 , 135, 90-98		22
1304	Interaction of menthol with mixed-lipid bilayer of stratum corneum: A coarse-grained simulation study. 2015 , 60, 98-107		23
1303	Biomembranes in atomistic and coarse-grained simulations. 2015 , 27, 323103		50
1302	Martini Coarse-Grained Force Field: Extension to DNA. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 3932-45	6.4	156
1301	Mechanical properties of carbon nanotube reinforced polymer nanocomposites: A coarse-grained model. 2015 , 80, 92-100		55
1300	MemProtMD: Automated Insertion of Membrane Protein Structures into Explicit Lipid Membranes. 2015 , 23, 1350-61		204
1299	Modeling Protein-Micelle Systems in Implicit Water. 2015 , 119, 8037-47		7
1298	Atomistic and Coarse Grain Topologies for the Cofactors Associated with the Photosystem II Core Complex. 2015 , 119, 7791-803		27
1297	Opening of the blood-brain barrier tight junction due to shock wave induced bubble collapse: a molecular dynamics simulation study. 2015 , 6, 1296-301		30
1296	Efficient Exploration of Membrane-Associated Phenomena at Atomic Resolution. 2015 , 248, 563-82		24
1295	Polarizable coarse-grained models for molecular dynamics simulation of liquid cyclohexane. 2015 , 36, 1311-21		7

1294	Preferred supramolecular organization and dimer interfaces of opioid receptors from simulated self-association. 2015 , 11, e1004148		55
1293	Automated parametrization of the coarse-grained Martini force field for small organic molecules. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2783-91	6.4	80
1292	The Flocculating Cationic Polypeptide from <i>Moringa oleifera</i> Seeds Damages Bacterial Cell Membranes by Causing Membrane Fusion. 2015 , 31, 4496-502		54
1291	Spontaneous adsorption of coiled-coil model peptides K and E to a mixed lipid bilayer. 2015 , 119, 4396-408		24
1290	Carboxylate Ion Pairing with Alkali-Metal Ions for β -Lactoglobulin and Its Role on Aggregation and Interfacial Adsorption. 2015 , 119, 5505-17		28
1289	Molecular dynamic simulation of Ca ²⁺ -ATPase interacting with lipid bilayer membrane. 2015 , 9, 85-94		2
1288	Development of a coarse-grained β -chitin model on the basis of MARTINI forcefield. 2015 , 21, 128		19
1287	Mechanisms of the self-assembly of EAK16-family peptides into fibrillar and globular structures: molecular dynamics simulations from nano- to micro-seconds. 2015 , 44, 263-76		15
1286	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
1285	Structural effects of tachyplesin I and its linear derivative on their aggregation and mobility in lipid bilayers. 2015 , 59, 123-8		5
1284	Cofilin reduces the mechanical properties of actin filaments: approach with coarse-grained methods. 2015 , 17, 8148-58		11
1283	Physics-Based Potentials for Coarse-Grained Modeling of Protein-DNA Interactions. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 1792-808	6.4	14
1282	Thermodynamic and kinetic characterization of transmembrane helix association. 2015 , 17, 1390-8		17
1281	Hybrid Quantum Mechanics/Molecular Mechanics/Coarse Grained Modeling: A Triple-Resolution Approach for Biomolecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 1809-18	6.4	30
1280	Mesosopic simulation of phospholipid membranes, peptides, and proteins with molecular fragment dynamics. 2015 , 55, 983-97		8
1279	Molecular Dynamics Simulations of Retrograde Condensation in Narrow Oil-Wet Nanopores.. 2015 , 119, 10040-10047		12
1278	Parametrization of Backbone Flexibility in a Coarse-Grained Force Field for Proteins (COFFDROP) Derived from All-Atom Explicit-Solvent Molecular Dynamics Simulations of All Possible Two-Residue Peptides. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2341-54	6.4	10
1277	Positively charged amino acids at the SNAP-25 C terminus determine fusion rates, fusion pore properties, and energetics of tight SNARE complex zippering. 2015 , 35, 3230-9		17

1276	Molecular dynamics simulations of GPCR-cholesterol interaction: An emerging paradigm. 2015 , 1848, 1775-82		103
1275	How ABA block polymers activate cytochrome c in toluene: molecular dynamics simulation and experimental observation. 2015 , 17, 10708-14		5
1274	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
1273	Multiscale modeling of nanomaterials. 2015 , 3-53		3
1272	Molecular Dynamics Simulations of a Binary Protein Mixture Adsorption onto Ion-Exchange Adsorbent. 2015 , 54, 2794-2802		7
1271	Synergistic effects of magainin 2 and PGLa on their heterodimer formation, aggregation, and insertion into the bilayer. 2015 , 5, 2047-2055		22
1270	Membrane targeting of the yeast exocyst complex. 2015 , 1848, 1481-9		36
1269	The Bacterial Hydrophobin BslA is a Switchable Ellipsoidal Janus Nanocolloid. 2015 , 31, 11558-63		22
1268	Structure and Dynamics of Intrinsically Disordered Proteins. 2015 , 870, 35-48		11
1267	Organization and Dynamics of Receptor Proteins in a Plasma Membrane. 2015 , 137, 14694-704		78
1266	Osmolyte Induced Changes in Peptide Conformational Ensemble Correlate with Slower Amyloid Aggregation: A Coarse-Grained Simulation Study. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5918-28	6.4	8
1265	Derivation of coarse-grained simulation models of chlorophyll molecules in lipid bilayers for applications in light harvesting systems. 2015 , 17, 22054-63		8
1264	Morphogenic Peptides in Regeneration of Load Bearing Tissues. 2015 , 881, 95-110		9
1263	Hydrophobic mismatch sorts SNARE proteins into distinct membrane domains. 2015 , 6, 5984		89
1262	Coarse-grained molecular dynamics studies of the translocation mechanism of polyarginines across asymmetric membrane under tension. 2015 , 5, 12808		26
1261	Liquid-liquid equilibria for soft-repulsive particles: improved equation of state and methodology for representing molecules of different sizes and chemistry in dissipative particle dynamics. 2015 , 142, 044902		19
1260	A Coarse-Grained Implicit Solvent Model for Poly(ethylene oxide), CnEm Surfactants, and Hydrophobically End-Capped Poly(ethylene oxide) and Its Application to Micelle Self-Assembly and Phase Behavior. 2015 , 48, 7709-7718		32
1259	Synaptobrevin Transmembrane Domain Dimerization Studied by Multiscale Molecular Dynamics Simulations. 2015 , 109, 760-71		17

1258	Multistep Molecular Dynamics Simulations Identify the Highly Cooperative Activity of Melittin in Recognizing and Stabilizing Membrane Pores. 2015 , 31, 9388-401		33
1257	Polysaccharide-Protein Complexes in a Coarse-Grained Model. 2015 , 119, 12028-41		31
1256	Adaptive resolution simulation of polarizable supramolecular coarse-grained water models. 2015 , 142, 244118		39
1255	Amphiphilic Peptides A6K and V6K Display Distinct Oligomeric Structures and Self-Assembly Dynamics: A Combined All-Atom and Coarse-Grained Simulation Study. 2015 , 16, 2940-9		29
1254	CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 4486-94	6.4	181
1253	Lipid insertion domain unfolding regulates protein orientational transition behavior in a lipid bilayer. 2015 , 206, 22-39		5
1252	Simulating Gram-Negative Bacterial Outer Membrane: A Coarse Grain Model. 2015 , 119, 14668-82		51
1251	SAFT-Force field for the simulation of molecular fluids: 4. A single-site coarse-grained model of water applicable over a wide temperature range. 2015 , 113, 1228-1249		63
1250	Multiscale Molecular Dynamics Simulations of Model Hydrophobically Modified Ethylene Oxide Urethane Micelles. 2015 , 119, 12540-51		12
1249	Molecular models of nanodiscs. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 4923-32	6.4	24
1248	Regulation of the Ca(2+)-ATPase by cholesterol: a specific or non-specific effect?. 2015 , 32, 75-87		11
1247	The Molecular Mechanism Underlying Recruitment and Insertion of Lipid-Anchored LC3 Protein into Membranes. 2015 , 109, 2067-78		22
1246	Properties of the polarizable MARTINI water model: A comparative study for aqueous electrolyte solutions. 2015 , 212, 103-110		23
1245	Transferability of the coarse-grained potentials for trans-1,4-polybutadiene. 2015 , 17, 31693-706		13
1244	Testing the transferability of a coarse-grained model to intrinsically disordered proteins. 2015 , 17, 31741-9		17
1243	SIRAH: a structurally unbiased coarse-grained force field for proteins with aqueous solvation and long-range electrostatics. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 723-39	6.4	84
1242	Interaction of cyclic and linear Labaditin peptides with anionic and zwitterionic micelles. 2015 , 438, 39-46		5
1241	Amphipathic membrane-active peptides recognize and stabilize ruptured membrane pores: exploring cause and effect with coarse-grained simulations. 2015 , 31, 752-61		19

1240	Interactions of the EGFR juxtamembrane domain with PIP2-containing lipid bilayers: Insights from multiscale molecular dynamics simulations. 2015 , 1850, 1017-1025	46
1239	Exploring the sequence space for (tri-)peptide self-assembly to design and discover new hydrogels. 2015 , 7, 30-7	445
1238	Chemically specific multiscale modeling of clay-polymer nanocomposites reveals intercalation dynamics, tactoid self-assembly and emergent materials properties. 2015 , 27, 966-84	83
1237	Enhanced Sampling of Coarse-Grained Transmembrane-Peptide Structure Formation from Hydrogen-Bond Replica Exchange. 2015 , 248, 395-405	10
1236	Biochemical Roles of Eukaryotic Cell Surface Macromolecules. 2015 ,	4
1235	Cholesterol behavior in asymmetric lipid bilayers: insights from molecular dynamics simulations. 2015 , 1232, 291-306	10
1234	A coarse-grained model for the mechanical behavior of multi-layer graphene. 2015 , 82, 103-115	118
1233	Molecular Modeling of Proteins. 2015 ,	6
1232	Methods in Membrane Lipids. 2015 ,	4
1231	Theoretical and computational investigations of nanoparticle-biomembrane interactions in cellular delivery. 2015 , 11, 1055-71	192
1230	Construction and validation of an atomic model for bacterial TSPO from electron microscopy density, evolutionary constraints, and biochemical and biophysical data. 2015 , 1848, 568-80	13
1229	Computational modeling of membrane proteins. 2015 , 83, 1-24	69
1228	Molecular dynamics methods to predict peptide locations in membranes: LAH4 as a stringent test case. 2015 , 1848, 581-92	33
1227	Theoretical insight into the relationship between the structures of antimicrobial peptides and their actions on bacterial membranes. 2015 , 119, 850-60	29
1226	Structural and Thermodynamic Insight into Spontaneous Membrane-Translocating Peptides Across Model PC/PG Lipid Bilayers. 2015 , 248, 505-15	13
1225	Experimental and computational investigation of the effect of hydrophobicity on aggregation and osteoinductive potential of BMP-2-derived peptide in a hydrogel matrix. 2015 , 21, 134-46	17
1224	Bioinformatics for Membrane Lipid Simulations: Models, Computational Methods, and Web Server Tools. 2016 ,	2
1223	Dynamics of the Large Progenitor Toxin Complex of Clostridium botulinum. 2016 , 09,	

1222	Mesoscale studies of ionic closed membranes with polyhedral geometries. 2016 , 4, 061102	2
1221	Impact of Lipid Composition and Receptor Conformation on the Spatio-temporal Organization of μ Opioid Receptors in a Multi-component Plasma Membrane Model. 2016 , 12, e1005240	40
1220	Multiscale Simulations Suggest a Mechanism for the Association of the Dok7 PH Domain with PIP-Containing Membranes. 2016 , 12, e1005028	20
1219	CLUB-MARTINI: Selecting Favourable Interactions amongst Available Candidates, a Coarse-Grained Simulation Approach to Scoring Docking Decoys. 2016 , 11, e0155251	13
1218	Membrane-Mediated Oligomerization of G Protein Coupled Receptors and Its Implications for GPCR Function. 2016 , 7, 494	72
1217	Effects of Concentrations on the Transdermal Permeation Enhancing Mechanisms of Borneol: A Coarse-Grained Molecular Dynamics Simulation on Mixed-Bilayer Membranes. 2016 , 17,	14
1216	Cardiolipin binds selectively but transiently to conserved lysine residues in the rotor of metazoan ATP synthases. 2016 , 113, 8687-92	80
1215	Sodium chloride's effect on self-assembly of diphenylalanine bilayer. 2016 , 37, 1839-46	7
1214	Pushing the Envelope: Dengue Viral Membrane Coaxed into Shape by Molecular Simulations. 2016 , 24, 1410-1420	32
1213	Kainate receptor pore-forming and auxiliary subunits regulate channel block by a novel mechanism. 2016 , 594, 1821-40	12
1212	Necessity of high-resolution for coarse-grained modeling of flexible proteins. 2016 , 37, 1725-33	5
1211	Performance of protein-structure predictions with the physics-based UNRES force field in CASP11. 2016 , 32, 3270-3278	36
1210	Membrane protein assembly: two cytoplasmic phosphorylated serine sites of Vpu from HIV-1 affect oligomerization. 2016 , 6, 28866	2
1209	Exocyst SEC3 and Phosphoinositides Define Sites of Exocytosis in Pollen Tube Initiation and Growth. 2016 , 172, 980-1002	53
1208	Steric hindrance of SNARE transmembrane domain organization impairs the hemifusion-to-fusion transition. 2016 , 17, 1590-1608	14
1207	Mechanism of Inhibition of Human Islet Amyloid Polypeptide-Induced Membrane Damage by a Small Organic Fluorogen. 2016 , 6, 21614	15
1206	The derivation and approximation of coarse-grained dynamics from Langevin dynamics. 2016 , 145, 204117	20
1205	Nanobubbles, cavitation, shock waves and traumatic brain injury. 2016 , 18, 32638-32652	21

1204	Membrane omega-3 fatty acids modulate the oligomerisation kinetics of adenosine A2A and dopamine D2 receptors. 2016 , 6, 19839		71
1203	Refining the treatment of membrane proteins by coarse-grained models. 2016 , 84, 92-117		25
1202	Exploring the Formation and the Structure of Synaptobrevin Oligomers in a Model Membrane. 2016 , 110, 2004-15		11
1201	Polymer Conjugation as a Strategy for Long-Range Order in Supramolecular Polymers. 2016 , 120, 3425-33		5
1200	Atomic-level description of protein-lipid interactions using an accelerated membrane model. 2016 , 1858, 1573-83		29
1199	Constructing Optimal Coarse-Grained Sites of Huge Biomolecules by Fluctuation Maximization. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2091-100	6.4	15
1198	A Direct Method for Incorporating Experimental Data into Multiscale Coarse-Grained Models. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2144-53	6.4	22
1197	Gold nanoparticles in model biological membranes: A computational perspective. 2016 , 1858, 2380-2389		43
1196	MARTINI Coarse-Grained Model of Triton TX-100 in Pure DPPC Monolayer and Bilayer Interfaces. 2016 , 120, 3821-32		14
1195	Improved Side Chain Dynamics in MARTINI Simulations of Protein-Lipid Interfaces. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2446-58	6.4	34
1194	Free Energy Landscape of Lipid Interactions with Regulatory Binding Sites on the Transmembrane Domain of the EGF Receptor. 2016 , 120, 8154-63		43
1193	Patch formation of a viral channel forming protein within a lipid membrane--Vpu of HIV-1. 2016 , 12, 1118-27		3
1192	Effect of lipid head group interactions on membrane properties and membrane-induced cationic β hairpin folding. 2016 , 18, 17836-50		15
1191	Biophysical characterization of cofilin-induced extension-torsion coupling in actin filaments. 2016 , 49, 1831-1835		2
1190	Effects of Transmembrane β Helix Length and Concentration on Phase Behavior in Four-Component Lipid Mixtures: A Molecular Dynamics Study. 2016 , 120, 4064-77		11
1189	Steered molecular dynamics analysis of the role of cofilin in increasing the flexibility of actin filaments. 2016 , 218, 27-35		8
1188	Coarse-grained simulations of hemolytic peptide β lysin interacting with a POPC bilayer. 2016 , 1858, 3182-3194		4
1187	Transferability of a coarse-grained atactic polystyrene model: the non-bonded potential effect. 2016 , 18, 29808-29824		17

- 1186 Interactions of Pleckstrin Homology Domains with Membranes: Adding Back the Bilayer via High-Throughput Molecular Dynamics. **2016**, 24, 1421-1431 51
- 1185 Interactions between C60 and vesicles: a coarse-grained molecular dynamics simulation. **2016**, 6, 90388-90396 4
- 1184 Defining a Physical Basis for Diversity in Protein Self-Assemblies Using a Minimal Model. **2016**, 138, 13911-13923 5
- 1183 The self-assembly mechanism of tetra-peptides from the motif of β -amyloid peptides: a combined coarse-grained and all-atom molecular dynamics simulation. **2016**, 6, 100072-100078 7
- 1182 Membrane Compartmentalization Reducing the Mobility of Lipids and Proteins within a Model Plasma Membrane. **2016**, 120, 8873-81 22
- 1181 Large-Conductance Transmembrane Porin Made from DNA Origami. **2016**, 10, 8207-14 124
- 1180 Interplay of Specific Trans- and Juxtamembrane Interfaces in Plexin A3 Dimerization and Signal Transduction. **2016**, 55, 4928-38 3
- 1179 Structural and Functional Basis for Lipid Synergy on the Activity of the Antibacterial Peptide ABC Transporter McjD. **2016**, 291, 21656-21668 22
- 1178 Membrane insertion of a Tc toxin in near-atomic detail. **2016**, 23, 884-890 67
- 1177 The Ebola virus protein VP40 hexamer enhances the clustering of PI(4,5)P lipids in the plasma membrane. **2016**, 18, 28409-28417 34
- 1176 DPPC-cholesterol phase diagram using coarse-grained Molecular Dynamics simulations. **2016**, 1858, 2846-2857 63
- 1175 Expanding the Nanoarchitectural Diversity Through Aromatic Di- and Tri-Peptide Coassembly: Nanostructures and Molecular Mechanisms. **2016**, 10, 8316-24 66
- 1174 Impact of membrane lipid composition on the structure and stability of the transmembrane domain of amyloid precursor protein. **2016**, 113, E5281-7 51
- 1173 The ganglioside GM1 interacts with the serotonin receptor via the sphingolipid binding domain. **2016**, 1858, 2818-2826 34
- 1172 Hybrid Dendrimers of PPI(core)-PAMAM(shell): A Molecular Dynamics Simulation Study. **2016**, 120, 9564-75 20
- 1171 How flexible is a protein: simple estimates using FRET microscopy. **2016**, 12, 2988-91 4
- 1170 Molecular aspects of the interaction between Mason-Pfizer monkey virus matrix protein and artificial phospholipid membrane. **2016**, 84, 1717-1727 3
- 1169 Lipid molecules can induce an opening of membrane-facing tunnels in cytochrome P450 1A2. **2016**, 18, 30344-30356 17

1168	Coarse-grained modeling of crystal growth and polymorphism of a model pharmaceutical molecule. 2016 , 12, 8246-8255		16
1167	Organization and Structure of Branched Amphipathic Oligopeptide Bilayers. 2016 , 32, 9883-91		6
1166	The role of natural processes and surface energy of inhaled engineered nanoparticles on aggregation and corona formation. 2016 , 2, 38-44		45
1165	Adaptive Resolution Simulation of Supramolecular Water: The Concurrent Making, Breaking, and Remaking of Water Bundles. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 4138-45	6.4	26
1164	Multiscale simulations on conformational dynamics and membrane interactions of the non-structural 2 (NS2) transmembrane domain. 2016 , 478, 193-198		4
1163	Conformational Changes in the Epidermal Growth Factor Receptor: Role of the Transmembrane Domain Investigated by Coarse-Grained MetaDynamics Free Energy Calculations. 2016 , 138, 10611-22		63
1162	Simulated Permeation and Characterization of PEGylated Gold Nanoparticles in a Lipid Bilayer System. 2016 , 32, 7541-55		19
1161	Understanding the curvature effect of silica nanoparticles on lysozyme adsorption orientation and conformation: a mesoscopic coarse-grained simulation study. 2016 , 18, 23500-7		40
1160	Systematic Generation of Anisotropic Coarse-Grained Lennard-Jones Potentials and Their Application to Ordered Soft Matter. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 4362-74	6.4	18
1159	Thermodynamics of cell-penetrating HIV1 TAT peptide insertion into PC/PS/CHOL model bilayers through transmembrane pores: the roles of cholesterol and anionic lipids. 2016 , 12, 6716-27		19
1158	Structure of Human Acid Sphingomyelinase Reveals the Role of the Saposin Domain in Activating Substrate Hydrolysis. 2016 , 428, 3026-42		34
1157	Atomistic Simulation of SolGel-Derived Hybrid Materials. 2016 , 1-34		
1156	Protein Crowding in Lipid Bilayers Gives Rise to Non-Gaussian Anomalous Lateral Diffusion of Phospholipids and Proteins. 2016 , 6,		110
1155	Multiscale Coarse-Graining of Polarizable Models through Force-Matched Dipole Fluctuations. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 5737-5750	6.4	10
1154	Protein-dependent Membrane Interaction of A Partially Disordered Protein Complex with Oleic Acid: Implications for Cancer Lipidomics. 2016 , 6, 35015		8
1153	Breaking a virus: Identifying molecular level failure modes of a viral capsid by multiscale modeling. 2016 , 225, 1757-1774		10
1152	Structure, Thermodynamics, and Folding Pathways for a Tryptophan Zipper as a Function of Local Rigidification. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 6109-6117	6.4	5
1151	The C-terminal Domains of Apoptotic BH3-only Proteins Mediate Their Insertion into Distinct Biological Membranes. 2016 , 291, 25207-25216		8

1150	MARTINI Coarse-Grained Model of Solid-Liquid Interface. 2016 , 120, 26259-26269	4
1149	Translocation mechanism of C60 and C60 derivations across a cell membrane. 2016 , 18, 1	6
1148	Single-molecule visualization of dynamic transitions of pore-forming peptides among multiple transmembrane positions. 2016 , 7, 12906	22
1147	Coarse-Grained Simulations of Membrane Insertion and Folding of Small Helical Proteins Using the CABS Model. 2016 , 56, 2207-2215	12
1146	TMFF-A Two-Bead Multipole Force Field for Coarse-Grained Molecular Dynamics Simulation of Protein. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 6147-6156	6.4 11
1145	Lipid-Loving ANTs: Molecular Simulations of Cardiolipin Interactions and the Organization of the Adenine Nucleotide Translocase in Model Mitochondrial Membranes. 2016 , 55, 6238-6249	52
1144	Coarse-Grained Models for Automated Fragmentation and Parametrization of Molecular Databases. 2016 , 56, 2361-2377	18
1143	A Multiscale Study on the Penetration Enhancement Mechanism of Menthol to Osthole. 2016 , 56, 2234-2242	11
1142	Concentration-induced structural transition of block polymer self-assemblies on a nanoparticle surface: computer simulation. 2016 , 6, 102057-102067	4
1141	The raspberry model for protein-like particles: Ellipsoids and confinement in cylindrical pores. 2016 , 225, 1643-1662	6
1140	Molecular characterization of a family 5 glycoside hydrolase suggests an induced-fit enzymatic mechanism. 2016 , 6, 23473	17
1139	Cholesterol-dependent Conformational Plasticity in GPCR Dimers. 2016 , 6, 31858	60
1138	Structural basis for the membrane association of ankyrinG via palmitoylation. 2016 , 6, 23981	12
1137	Anomalous Dynamics of a Lipid Recognition Protein on a Membrane Surface. 2015 , 5, 18245	34
1136	Description and control of dissociation channels in gas-phase protein complexes. 2016 , 145, 065101	5
1135	Computational Theory. 2016 , 31-42	
1134	A Discontinuous Potential Model for Protein-Protein Interactions. 2016 , 2016, 1-20	
1133	Gating mechanism of mechanosensitive channel of large conductance: a coupled continuum mechanical-continuum solvation approach. 2016 , 15, 1557-1576	10

1132	Coarse-Grained Simulations of Heme Proteins: Validation and Study of Large Conformational Transitions. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 3390-7	6.4	8
1131	Molecular dynamics simulations and structure-based network analysis reveal structural and functional aspects of G-protein coupled receptor dimer interactions. 2016 , 30, 489-512		22
1130	Coarse-Grained Protein Models and Their Applications. 2016 , 116, 7898-936		489
1129	Simulating the interaction of lipid membranes with polymer and ligand-coated nanoparticles. 2016 , 1, 276-296		17
1128	Amyloid and Amyloid Fibrils. 2016 , 1-30		
1127	Adsorption of Plasma Proteins onto PEGylated Lipid Bilayers: The Effect of PEG Size and Grafting Density. 2016 , 17, 1757-65		48
1126	Optimizing the Multivalent Binding of the Bacterial Lectin LecA by Glycopeptide Dendrimers for Therapeutic Purposes. 2016 , 56, 1193-204		7
1125	Protein-Backbone Thermodynamics across the Membrane Interface. 2016 , 120, 6391-400		6
1124	Molecular dynamics simulation and bioinformatics study on chloroplast stromal ridge complex from rice (<i>Oryza sativa</i> L.). 2016 , 17, 28		8
1123	A Eukaryotic Sensor for Membrane Lipid Saturation. 2016 , 63, 49-59		75
1122	Evaluation of the coarse-grained OPEP force field for protein-protein docking. 2016 , 9, 4		19
1121	The mystery of the fusion pore. 2016 , 23, 5-6		13
1120	Properties of Poloxamer Molecules and Poloxamer Micelles Dissolved in Water and Next to Lipid Bilayers: Results from Computer Simulations. 2016 , 120, 5823-30		38
1119	A non-zipper-like tetrameric coiled coil promotes membrane fusion. 2016 , 6, 7990-7998		17
1118	What can simulations tell us about GPCRs: Integrating the scales. 2016 , 132, 429-52		16
1117	Force Field Development for Lipid Membrane Simulations. 2016 , 1858, 2483-2497		73
1116	Association of Peripheral Membrane Proteins with Membranes: Free Energy of Binding of GRP1 PH Domain with Phosphatidylinositol Phosphate-Containing Model Bilayers. 2016 , 7, 1219-24		34
1115	Molecular mechanism of cardiolipin-mediated assembly of respiratory chain supercomplexes. 2016 , 7, 4435-4443		57

1114	Experimental and simulation studies of polyarginines across the membrane of giant unilamellar vesicles. 2016 , 6, 30454-30459	7
1113	A Molecular Look at Membranes. 2016 , 77, 1-25	3
1112	The Role of the Membrane in the Structure and Biophysical Robustness of the Dengue Virion Envelope. 2016 , 24, 375-82	62
1111	Vesicle Geometries Enabled by Dynamically Trapped States. 2016 , 10, 2287-94	8
1110	Interaction of peptides with cell membranes: insights from molecular modeling. 2016 , 28, 083001	10
1109	Structures of the EphA2 Receptor at the Membrane: Role of Lipid Interactions. 2016 , 24, 337-47	27
1108	Molecular Architecture of the Blood Brain Barrier Tight Junction Proteins--A Synergistic Computational and In Vitro Approach. 2016 , 120, 77-88	28
1107	Molecular dynamics simulation of coarse-grained poly(L-lysine) dendrimers. 2016 , 22, 59	21
1106	Membrane remodeling and mechanics: Experiments and simulations of β -Synuclein. 2016 , 1858, 1594-609	32
1105	Membrane-Anchored Cytochrome P450 1A2-Cytochrome b5 Complex Features an X-Shaped Contact between Antiparallel Transmembrane Helices. 2016 , 29, 626-36	7
1104	Efficient preparation and analysis of membrane and membrane protein systems. 2016 , 1858, 2468-2482	23
1103	Hybrid particle-field molecular dynamics simulation for polyelectrolyte systems. 2016 , 18, 9799-808	21
1102	Simulations of inorganic-bioorganic interfaces to discover new materials: insights, comparisons to experiment, challenges, and opportunities. 2016 , 45, 412-48	143
1101	Anisotropic Membrane Curvature Sensing by Amphipathic Peptides. 2016 , 110, 197-204	32
1100	Effects of protein crowding on membrane systems. 2016 , 1858, 2441-2450	66
1099	P-Type ATPases. 2016 ,	3
1098	Computer modelling of the surface tension of the gas-liquid and liquid-liquid interface. 2016 , 45, 1387-409	121
1097	CG2AA: backmapping protein coarse-grained structures. 2016 , 32, 1235-7	32

1096	Ibuprofen loading and release in amphiphilic peptide FA32 and its derivatives: a coarse-grained molecular dynamics simulation study. 2016 , 42, 679-687	8
1095	Refinement of a coarse-grained model of poly(2,6-dimethyl-1,4-phenylene ether) and its application to blends of PPE and PS. 2016 , 42, 312-320	2
1094	Reduced point charge models of proteins: assessment based on molecular dynamics simulations. 2016 , 42, 289-304	3
1093	Interaction of chemokine receptor CXCR4 in monomeric and dimeric state with its endogenous ligand CXCL12: coarse-grained simulations identify differences. 2017 , 35, 399-412	11
1092	Application of Monte Carlo simulation in addressing key issues of complex coacervation formed by polyelectrolytes and oppositely charged colloids. 2017 , 239, 31-45	12
1091	The dynamic binding of cholesterol to the multiple sites of C99: as revealed by coarse-grained and all-atom simulations. 2017 , 19, 3845-3856	9
1090	Further understanding of the biased diffusion for peptide adsorption on uncharged solid surfaces that strongly interact with water molecules. 2017 , 518, 197-207	3
1089	Effects of Concentration and Ionization Degree of Anchoring Cationic Polymers on the Lateral Heterogeneity of Anionic Lipid Monolayers. 2017 , 121, 984-994	5
1088	Enhanced Computational Sampling of Perylene and Peryloothiophene Packing with Rigid-Body Models. 2017 , 2, 353-362	10
1087	A framework for multi-scale simulation of crystal growth in the presence of polymers. 2017 , 13, 1904-1913	14
1086	Structural effects and translocation of spontaneous membrane-translocating peptides with POPC bilayer. 2017 , 16, 1750002	1
1085	High-Throughput Simulations Reveal Membrane-Mediated Effects of Alcohols on MscL Gating. 2017 , 139, 2664-2671	24
1084	Performance Comparison of Systematic Methods for Rigorous Definition of Coarse-Grained Sites of Large Biomolecules. 2017 , 57, 214-222	5
1083	Coarse-Grained Molecular Simulation of the Hierarchical Self-Assembly of π -Conjugated Optoelectronic Peptides. 2017 , 121, 1684-1706	26
1082	Protein Aggregation and Molecular Crowding: Perspectives From Multiscale Simulations. 2017 , 329, 49-77	16
1081	Structural Insights How PIP2 Imposes Preferred Binding Orientations of FAK at Lipid Membranes. 2017 , 121, 3523-3535	17
1080	Evaluation of the hybrid resolution PACE model for the study of folding, insertion, and pore formation of membrane associated peptides. 2017 , 38, 1462-1471	16
1079	Interaction of Scots Pine Defensin with Model Membrane by Coarse-Grained Molecular Dynamics. 2017 , 250, 205-216	9

1078	Protein simulation using coarse-grained two-bead multipole force field with polarizable water models. 2017 , 146, 065101		2
1077	Computing the Rotational Diffusion of Biomolecules via Molecular Dynamics Simulation and Quaternion Orientations. 2017 , 121, 1812-1823		16
1076	Combining the MARTINI and Structure-Based Coarse-Grained Approaches for the Molecular Dynamics Studies of Conformational Transitions in Proteins. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 1366-1374	6.4	70
1075	Two-bead polarizable water models combined with a two-bead multipole force field (TMFF) for coarse-grained simulation of proteins. 2017 , 19, 7410-7419		7
1074	Bulk Heterojunction Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations. 2017 , 139, 3697-3705		99
1073	Self-assembling study of sarcolipin and its mutants in multiple molecular dynamic simulations. 2017 , 85, 1065-1077		4
1072	Dynamic interactions between a membrane binding protein and lipids induce fluctuating diffusivity. 2017 , 3, e1601871		40
1071	Computational Prediction of the Heterodimeric and Higher-Order Structure of gpE1/gpE2 Envelope Glycoproteins Encoded by Hepatitis C Virus. 2017 , 91,		24
1070	Discrete Molecular Dynamics Approach to the Study of Disordered and Aggregating Proteins. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 1454-1461	6.4	14
1069	Biomimetic Phospholipid Membrane Organization on Graphene and Graphene Oxide Surfaces: A Molecular Dynamics Simulation Study. 2017 , 11, 1613-1625		54
1068	A refined polarizable water model for the coarse-grained MARTINI force field with long-range electrostatic interactions. 2017 , 146, 054501		47
1067	β-Synuclein's Uniquely Long Amphipathic Helix Enhances its Membrane Binding and Remodeling Capacity. 2017 , 250, 183-193		16
1066	Molecular dynamics simulations reveal how characteristics of surface and permeant affect permeation events at the surface of soft matter. 2017 , 43, 439-466		9
1065	Estimating the Lipophobic Contributions in Model Membranes. 2017 , 121, 2111-2120		5
1064	Line Tension Controls Liquid-Disordered ↔ Liquid-Ordered Domain Size Transition in Lipid Bilayers. 2017 , 112, 1431-1443		49
1063	Influence of membrane composition on the binding and folding of a membrane lytic peptide from the non-enveloped flock house virus. 2017 , 1859, 1190-1199		10
1062	Lipid Flip-Flop and Pore Nucleation on Zwitterionic Bilayers are Asymmetric under Ionic Imbalance. 2017 , 13, 1603708		8
1061	A general method for the derivation of the functional forms of the effective energy terms in coarse-grained energy functions of polymers. I. Backbone potentials of coarse-grained polypeptide chains. 2017 , 146, 124106		31

1060	Supramolecular nanoparticles of calcitonin and dipeptide for long-term controlled release. 2017 , 256, 182-192	22
1059	Structural features and lipid binding domain of tubulin on biomimetic mitochondrial membranes. 2017 , 114, E3622-E3631	30
1058	Entropic forces drive self-organization and membrane fusion by SNARE proteins. 2017 , 114, 5455-5460	32
1057	How a short pore forming peptide spans the lipid membrane. 2017 , 12, 02D405	3
1056	Multiscale simulations for understanding the evolution and mechanism of hierarchical peptide self-assembly. 2017 , 19, 23614-23631	37
1055	Molecular Basis for Mitochondrial Signaling. 2017 ,	3
1054	Adsorption of plasma proteins onto PEGylated single-walled carbon nanotubes: The effects of protein shape, PEG size and grafting density. 2017 , 75, 1-8	7
1053	Testing High Concentrations of Membrane Active Antibiotic Chlorhexidine Via Computational Titration and Calorimetry. 2017 , 121, 4657-4668	3
1052	Molecular Time-machines to unravel key biological events for drug design. 2017 , 7, e1306	7
1051	Aggregation of thrombin-derived C-terminal fragments as a previously undisclosed host defense mechanism. 2017 , 114, E4213-E4222	37
1050	Effects of the asphaltene structure and the tetralin/heptane solvent ratio on the size and shape of asphaltene aggregates. 2017 , 19, 13931-13940	10
1049	Interplay of G Protein-Coupled Receptors with the Membrane: Insights from Supra-Atomic Coarse Grain Molecular Dynamics Simulations. 2017 , 117, 156-185	42
1048	Rational Design of a Transferrin-Binding Peptide Sequence Tailored to Targeted Nanoparticle Internalization. 2017 , 28, 471-480	48
1047	Martini Coarse-Grained Force Field: Extension to RNA. 2017 , 113, 246-256	74
1046	Looking "Under the Hood" of Cellular Mechanotransduction with Computational Tools: A Systems Biomechanics Approach across Multiple Scales. 2017 , 3, 2712-2726	8
1045	Control of the hierarchical assembly of E-conjugated optoelectronic peptides by pH and flow. 2017 , 15, 5484-5502	14
1044	Structural Behavior of the Peptaibol Harzianin HK VI in a DMPC Bilayer: Insights from MD Simulations. 2017 , 112, 2602-2614	5
1043	Intrinsic map dynamics exploration for uncharted effective free-energy landscapes. 2017 , 114, E5494-E5503	72

1042	Structure Formation in Langmuir Peptide Films As Revealed from Coarse-Grained Molecular Dynamics Simulations. 2017 , 33, 6492-6502		4
1041	Computational studies of peptide-induced membrane pore formation. 2017 , 372,		28
1040	Asymmetric osmotic water permeation through a vesicle membrane. 2017 , 146, 204902		6
1039	Insights into the transmembrane helix associations of kit ligand by molecular dynamics simulation and TOXCAT. 2017 , 85, 1362-1370		3
1038	Molecular Simulations of Complex Membrane Models. 2017 , 1-18		
1037	An Ensemble-Based Protocol for the Computational Prediction of Helix-Helix Interactions in G Protein-Coupled Receptors using Coarse-Grained Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 2254-2270	6.4	21
1036	Interplay between Conformational Heterogeneity and Hydration in the Folding Landscape of a Designed Three-Helix Bundle. 2017 , 121, 2731-2738		2
1035	Switchable Redox Chemistry of the Hexameric Tyrosine-Coordinated Heme Protein. 2017 , 121, 3955-3964		5
1034	Selective ion binding and transport by membrane proteins [A computational perspective. 2017 , 345, 108-136		27
1033	Method for Developing Optical Sensors Using a Synthetic Dye-Fluorescent Protein FRET Pair and Computational Modeling and Assessment. 2017 , 1596, 89-99		1
1032	A BEST example of channel structure annotation by molecular simulation. 2017 , 11, 347-353		19
1031	Concentration Dependent Self-Assembly of TrK-NGF Receptor Derived Tripeptide: New Insights from Experiment and Computer Simulations. 2017 , 121, 815-824		20
1030	From Cooperative Self-Assembly to Water-Soluble Supramolecular Polymers Using Coarse-Grained Simulations. 2017 , 11, 1000-1011		56
1029	Influence of Monovalent Cation Size on Nanodomain Formation in Anionic-Zwitterionic Mixed Bilayers. 2017 , 121, 787-799		9
1028	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force of the Interaction of Amino Acid Side Chains in Water. VII. Charged-Hydrophobic/Polar and Polar-Hydrophobic/Polar Side Chains. 2017 , 121, 379-390		16
1027	Beneficial roles of H-donors as diluent and H-shuttle for asphaltenes in catalytic upgrading of vacuum residue. 2017 , 314, 1-10		34
1026	Thermodynamics of Hydrophobic Amino Acids in Solution: A Combined Experimental-Computational Study. 2017 , 8, 347-351		4
1025	Lipid and Peptide Diffusion in Bilayers: The Saffman-Delbrück Model and Periodic Boundary Conditions. 2017 , 121, 3443-3457		69

1024	Structure and lipid-binding properties of the kindlin-3 pleckstrin homology domain. 2017 , 474, 539-556	30
1023	The application of nonlocal theory method in the coarse-grained molecular dynamics simulations of long-chain polylactic acid. 2017 , 30, 630-637	8
1022	A tethering complex drives the terminal stage of SNARE-dependent membrane fusion. 2017 , 551, 634-638	67
1021	Smoothing potential energy surface of proteins by hybrid coarse grained approach. 2017 , 26, 050202	4
1020	Role of Bioinformatics in the Study of Ionic Channels. 2017 , 227, 17-37	1
1019	Hybrid All-Atom/Coarse-Grained Simulations of Proteins by Direct Coupling of CHARMM and PRIMO Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 5753-5765	6.4 23
1018	In silico screening of drug-membrane thermodynamics reveals linear relations between bulk partitioning and the potential of mean force. 2017 , 147, 125101	31
1017	pH-Induced interfacial properties of Chaplin E from <i>Streptomyces coelicolor</i> . 2017 , 160, 589-597	1
1016	Diffusion of Integral Membrane Proteins in Protein-Rich Membranes. 2017 , 8, 4308-4313	41
1015	Modeling the Self-Assembly of Bolaamphiphiles under Nanoconfinement by Coarse-Grained Molecular Dynamics. 2017 , 121, 8984-8990	5
1014	Adaptive resolution simulations of biomolecular systems. 2017 , 46, 821-835	16
1013	Thermodynamic Origin of Multilayer Structures in Langmuir Polymer Films. 2017 , 33, 11399-11405	
1012	Light-independent phospholipid scramblase activity of bacteriorhodopsin from <i>Halobacterium salinarum</i> . 2017 , 7, 9522	14
1011	Effects of Periplasmic Chaperones and Membrane Thickness on BamA-Catalyzed Outer-Membrane Protein Folding. 2017 , 429, 3776-3792	49
1010	Cardiolipin mediates membrane and channel interactions of the mitochondrial TIM23 protein import complex receptor Tim50. 2017 , 3, e1700532	34
1009	Insight of Transmembrane Processes of Self-Assembling Nanotubes Based on a Cyclic Peptide Using Coarse Grained Molecular Dynamics Simulation. 2017 , 121, 9006-9012	3
1008	In vitro blood cell viability profiling of polymers used in molecular assembly. 2017 , 7, 9481	58
1007	Biomembrane solubilization mechanism by Triton X-100: a computational study of the three stage model. 2017 , 19, 29780-29794	23

1006	Coarse-grained molecular dynamics studies of the structure and stability of peptide-based drug amphiphile filaments. 2017 , 13, 7721-7730	14
1005	Effects of Coarse Graining and Saturation of Hydrocarbon Chains on Structure and Dynamics of Simulated Lipid Molecules. 2017 , 7, 11476	11
1004	Multiple interactions between an Arf/GEF complex and charged lipids determine activation kinetics on the membrane. 2017 , 114, 11416-11421	27
1003	Multiscale molecular dynamics simulations of lipid interactions with P-glycoprotein in a complex membrane. 2017 , 77, 250-258	5
1002	Molecular dynamics exploration of poration and leaking caused by Kalata B1 in HIV-infected cell membrane compared to host and HIV membranes. 2017 , 7, 3638	7
1001	Biocompatible and blood-brain barrier permeable carbon dots for inhibition of A β fibrillation and toxicity, and BACE1 activity. 2017 , 9, 12862-12866	41
1000	Membrane Binding of Recoverin: From Mechanistic Understanding to Biological Functionality. 2017 , 3, 868-874	12
999	The mesoscopic membrane with proteins (MesM-P) model. 2017 , 147, 044101	14
998	Rationally designed peptide nanosponges for cell-based cancer therapy. 2017 , 13, 2555-2564	8
997	A Molecular Dynamics Study of the Short-Helical-Cytolytic Peptide Assembling and Bioactive on Membrane Interface. 2017 , 121, 17263-17275	4
996	Effect of lipid shape on toroidal pore formation and peptide orientation in lipid bilayers. 2017 , 19, 21340-21349	11
995	Interaction of hydrophobic polymers with model lipid bilayers. 2017 , 7, 6357	40
994	CHARMM-GUI Martini Maker for modeling and simulation of complex bacterial membranes with lipopolysaccharides. 2017 , 38, 2354-2363	77
993	Overcoming the Limitations of the MARTINI Force Field in Simulations of Polysaccharides. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 5039-5053	6.4 47
992	Maximum Likelihood Calibration of the UNRES Force Field for Simulation of Protein Structure and Dynamics. 2017 , 57, 2364-2377	33
991	Molecular Structuring and Phase Transition of Lipid-Based Formulations upon Water Dispersion: A Coarse-Grained Molecular Dynamics Simulation Approach. 2017 , 14, 4145-4153	13
990	Development of new coarse-grained models for chromonic liquid crystals: insights from top-down approaches. 2017 , 1-11	7
989	t-SNARE Transmembrane Domain Clustering Modulates Lipid Organization and Membrane Curvature. 2017 , 139, 18440-18443	10

988	The orientation and stability of the GPCR-Arrestin complex in a lipid bilayer. 2017 , 7, 16985	9
987	Effect of ergosterol on the fungal membrane properties. All-atom and coarse-grained molecular dynamics study. 2017 , 209, 45-53	13
986	Protein crowding and lipid complexity influence the nanoscale dynamic organization of ion channels in cell membranes. 2017 , 7, 16647	48
985	HyRes: a coarse-grained model for multi-scale enhanced sampling of disordered protein conformations. 2017 , 19, 32421-32432	13
984	Parameterization of Palmitoylated Cysteine, Farnesylated Cysteine, Geranylgeranylated Cysteine, and Myristoylated Glycine for the Martini Force Field. 2017 , 121, 11132-11143	13
983	Molecular dynamics simulation studies of transmembrane transport of chemical components in Chinese herbs and the function of platycodin D in a biological membrane. 2017 , 4, 174-183	2
982	"Martinizing" the Variational Implicit Solvent Method (VISM): Solvation Free Energy for Coarse-Grained Proteins. 2017 , 121, 6538-6548	8
981	Theory of wavelet-based coarse-graining hierarchies for molecular dynamics. 2017 , 96, 013301	1
980	Developing structure and thermodynamic properties-consistent coarse-grained model for random copolymer systems. 2017 , 123, 107-120	8
979	JED: a Java Essential Dynamics Program for comparative analysis of protein trajectories. 2017 , 18, 271	9
978	Efficient estimation of binding free energies between peptides and an MHC class II molecule using coarse-grained molecular dynamics simulations with a weighted histogram analysis method. 2017 , 38, 2007-2019	14
977	Membrane localization and dynamics of geranylgeranylated Rab5 hypervariable region. 2017 , 1859, 1335-1349	13
976	Polyunsaturated chains in asymmetric lipids disorder raft mixtures and preferentially associate with β -Synuclein. 2017 , 1859, 529-536	9
975	High-Resolution Coarse-Grained Model of Hydrated Anion-Exchange Membranes that Accounts for Hydrophobic and Ionic Interactions through Short-Ranged Potentials. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 245-264	6.4 22
974	Multiscale molecular dynamics simulation approaches to the structure and dynamics of viruses. 2017 , 128, 121-132	20
973	Advances in Molecular Modeling of Nanoparticle-Nucleic Acid Interfaces. 2017 , 28, 3-10	19
972	Optimal allosteric stabilization sites using contact stabilization analysis. 2017 , 38, 1138-1146	1
971	Convergence and Sampling in Determining Free Energy Landscapes for Membrane Protein Association. 2017 , 121, 3364-3375	69

970	Rotational behaviour of PEGylated gold nanorods in a lipid bilayer system. 2017 , 115, 1122-1143	12
969	Lipid perturbation by membrane proteins and the lipophobic effect. 2017 , 1859, 126-134	12
968	The Integrin Receptor in Biologically Relevant Bilayers: Insights from Molecular Dynamics Simulations. 2017 , 250, 337-351	17
967	Organic/Inorganic interface simulation for new material discoveries. 2017 , 7, e1277	7
966	Simulation study of interaction mechanism between peptide and asymmetric membrane. 2017 , 43, 34-41	5
965	CHARMM-GUI 10 years for biomolecular modeling and simulation. 2017 , 38, 1114-1124	119
964	The IM30/Vipp1 C-terminus associates with the lipid bilayer and modulates membrane fusion. 2017 , 1858, 126-136	20
963	Molecular Dynamics of Photosystem II Embedded in the Thylakoid Membrane. 2017 , 121, 3237-3249	23
962	The influence of curvature on the properties of the plasma membrane. Insights from atomistic molecular dynamics simulations. 2017 , 7, 16078	45
961	Comparison of coarse-grained (MARTINI) and atomistic molecular dynamics simulations of (alpha) and (beta) toxin nanopores in lipid membranes. 2017 , 129, 1017-1030	14
960	Membrane-Active Properties of an Amphitropic Peptide from the CyaA Toxin Translocation Region. 2017 , 9,	13
959	Regulation of Exocytotic Fusion Pores by SNARE Protein Transmembrane Domains. 2017 , 10, 315	23
958	Transferability of Polymer Chain Properties between Coarse-Grained and Atomistic Models of Natural Rubber Molecule Validated by Molecular Dynamics Simulations. 2017 , 901, 012096	2
957	Advances in Molecular Simulation. 2017 , 14-33	1
956	Phospholipids in chocolate: Structural insights and mechanistic explanations of rheological behavior by coarse-grained molecular dynamics simulations. 2018 , 228, 118-127	7
955	Cholesterol binding to a conserved site modulates the conformation, pharmacology, and transport kinetics of the human serotonin transporter. 2018 , 293, 3510-3523	33
954	In Silico Investigations of Calcium Phosphate Mineralization in Extracellular Vesicles. 2018 , 122, 3782-3789	6
953	GhoT of the GhoT/GhoS toxin/antitoxin system damages lipid membranes by forming transient pores. 2018 , 497, 467-472	6

952	Multiscale modeling of keratin, collagen, elastin and related human diseases: Perspectives from atomistic to coarse-grained molecular dynamics simulations. 2018 , 20, 112-124		19
951	Structure and Relaxation in Solutions of Monoclonal Antibodies. 2018 , 122, 2867-2880		23
950	Multiscale Coarse-Graining with Effective Polarizabilities: A Fully Bottom-Up Approach. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 1873-1886	6.4	3
949	Exploring GPCR-Lipid Interactions by Molecular Dynamics Simulations: Excitements, Challenges, and the Way Forward. 2018 , 122, 5727-5737		50
948	Molecular simulations of self-assembling bio-inspired supramolecular systems and their connection to experiments. 2018 , 47, 3470-3489		72
947	Materials-by-Design: Computation, Synthesis, and Characterization from Atoms to Structures. 2018 , 93,		23
946	Interaction of lecithin:cholesterol acyltransferase with lipid surfaces and apolipoprotein A-I-derived peptides. 2018 , 59, 670-683		8
945	A coarse grained molecular dynamics simulation study on the structural properties of carbon nanotube-dendrimer composites. 2018 , 14, 3151-3163		13
944	Structure and Dynamics of Solvated Polymers near a Silica Surface: On the Different Roles Played by Solvent. 2018 , 122, 4573-4582		6
943	Seeding and cross-seeding fibrillation of N-terminal prion protein peptides PrP(120-144). 2018 , 27, 1304-1313		8
942	The dimerization of PSGL-1 is driven by the transmembrane domain via a leucine zipper motif. 2018 , 86, 844-852		
941	How Does the Surface Tension Depend on the Surface Area with Coarse-Grained Models?. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 2644-2651	6.4	10
940	Cardiolipin dynamics and binding to conserved residues in the mitochondrial ADP/ATP carrier. 2018 , 1860, 1035-1045		30
939	Predicting ligand binding poses for low-resolution membrane protein models: Perspectives from multiscale simulations. 2018 , 498, 366-374		19
938	Molecular simulation aspects of amyloid peptides at membrane interface. 2018 , 1860, 1906-1916		23
937	Employing multi-GPU power for molecular dynamics simulation: an extension of GALAMOST. 2018 , 116, 1065-1077		23
936	The interfacial electrostatic potential modulates the insertion of cell-penetrating peptides into lipid bilayers. 2018 , 20, 5180-5189		19
935	A sumatriptan coarse-grained model to explore different environments: interplay with experimental techniques. 2018 , 47, 561-571		9

934	Coarse-Grained Molecular Simulation Model for Gecko Feet Keratin. 2018 , 122, 2203-2212		7
933	Communication between the leaflets of asymmetric membranes revealed from coarse-grain molecular dynamics simulations. 2018 , 8, 1805		21
932	Coarse-grained molecular dynamics simulations reveal lipid access pathways in P-glycoprotein. 2018 , 150, 417-429		18
931	Markov-state model for CO binding with carbonic anhydrase under confinement. 2018 , 148, 035101		3
930	Understanding carbon nanotube channel formation in the lipid membrane. 2018 , 29, 115702		2
929	Multiscale molecular dynamics simulations of lipid interactions with P-glycoprotein in a complex membrane. 2018 , 80, 147-156		21
928	Coarse-Grained Molecular Dynamics Force-Field for Polyacrylamide in Infinite Dilution Derived from Iterative Boltzmann Inversion and MARTINI Force-Field. 2018 , 122, 1516-1524		11
927	Modes of Interaction of Pleckstrin Homology Domains with Membranes: Toward a Computational Biochemistry of Membrane Recognition. 2018 , 430, 372-388		28
926	GADDLE Maps: General Algorithm for Discrete Object Deformations Based on Local Exchange Maps. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 466-478	6.4	5
925	Dynamics of OmpF Trimer Formation in the Bacterial Outer Membrane of Escherichia coli. 2018 , 34, 5623-5634		11
924	Hybrid Particle-Field Model for Conformational Dynamics of Peptide Chains. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 1120-1130	6.4	15
923	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. 2018 , 118, 4177-4338		235
922	Ab Initio Prediction of NMR Spin Relaxation Parameters from Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 1009-1019	6.4	18
921	Interaction of monomeric Ebola VP40 protein with a plasma membrane: A coarse-grained molecular dynamics (CGMD) simulation study. 2018 , 82, 137-144		2
920	Distinctive phosphoinositide- and Ca-binding properties of normal and cognitive performance-linked variant forms of KIBRA C2 domain. 2018 , 293, 9335-9344		5
919	Effect of Surface Charge and Hydrophobicity on Phospholipid-Nanoparticle Corona Formation: A Molecular Dynamics Simulation Study. 2018 , 25, 7-11		13
918	Protein Partitioning into Ordered Membrane Domains: Insights from Simulations. 2018 , 114, 1936-1944		32
917	Molecular Dynamics of the Association of L-Selectin and FERM Regulated by PIP2. 2018 , 114, 1858-1868		17

916	Penetration of antimicrobial peptides in a lung surfactant model. 2018 , 167, 345-353	17
915	Antimicrobial action of the cationic peptide, chrysopsin-3: a coarse-grained molecular dynamics study. 2018 , 14, 2796-2807	11
914	Structural Polymorphism in a Self-Assembled Tri-Aromatic Peptide System. 2018 , 12, 3253-3262	50
913	Structures of monomeric and oligomeric forms of the perforin-like protein 1. 2018 , 4, eaaq0762	20
912	Looking at the Disordered Proteins through the Computational Microscope. 2018 , 4, 534-542	27
911	Molecular Dynamics Modeling of Methylene Blue-DOPC Lipid Bilayer Interactions. 2018 , 34, 4314-4323	13
910	Designing phenylalanine-based hybrid biological materials: controlling morphology via molecular composition. 2018 , 16, 2499-2507	6
909	Design of Polyphosphate Inhibitors: A Molecular Dynamics Investigation on Polyethylene Glycol-Linked Cationic Binding Groups. 2018 , 19, 1358-1367	7
908	Nanopatterns of Phospholipid Assemblies on Carbon Nanotubes: A Molecular Dynamics Simulation Study. 2018 , 122, 7455-7463	3
907	Electronic Conductivity in Biomimetic Helical Peptide Nanofibers and Gels. 2018 , 12, 2652-2661	44
906	Cross-linked self-assembling peptide scaffolds. 2018 , 11, 586-602	28
905	Comparison of mechanistic transport cycle models of ABC exporters. 2018 , 1860, 818-832	66
904	Shielding effect in protein folding. 2018 , 79, 118-132	4
903	Molecular dynamics simulation strategies for designing carbon-nanotube-based targeted drug delivery. 2018 , 23, 235-250	58
902	Finding the needle in the haystack: towards solving the protein-folding problem computationally. 2018 , 53, 1-28	23
901	Coarse-grained molecular dynamics simulation of interactions between cyclic lipopeptide Bacillomycin D and cell membranes. 2018 , 44, 364-376	4
900	Recent Advances in Computational Approaches for Designing Potential Anti-Alzheimer's Agents. 2018 , 25-59	2
899	The effect of mutations in the lid region of <i>Thermomyces lanuginosus</i> lipase on interactions with triglyceride surfaces: A multi-scale simulation study. 2018 , 211, 4-15	14

898	Efficient potential of mean force calculation from multiscale simulations: Solute insertion in a lipid membrane. 2018 , 498, 282-287	14
897	Branched peptides integrate into self-assembled nanostructures and enhance biomechanics of peptidic hydrogels. 2018 , 66, 258-271	26
896	A Membrane Burial Potential with H-Bonds and Applications to Curved Membranes and Fast Simulations. 2018 , 115, 1872-1884	5
895	Modeling of Protein Structural Flexibility and Large-Scale Dynamics: Coarse-Grained Simulations and Elastic Network Models. 2018 , 19,	37
894	Intracellular Membrane Trafficking: Modeling Local Movements in Cells. 2018 , 259-301	2
893	Cell Movement. 2018 ,	2
892	Towards a molecular basis of ubiquitin signaling: A dual-scale simulation study of ubiquitin dimers. 2018 , 14, e1006589	15
891	Enriched Conformational Sampling of DNA and Proteins with a Hybrid Hamiltonian Derived from the Protein Data Bank. 2018 , 19,	3
890	Domain rearrangement and denaturation in Ebola virus protein VP40. 2018 , 8, 125129	7
889	Biochemical and Biophysical Roles of Cell Surface Molecules. 2018 ,	1
888	Molecular Signatures of Cholesterol Interaction with Serotonin Receptors. 2018 , 1112, 151-160	4
887	Structural Model of the mIgM B-Cell Receptor Transmembrane Domain From Self-Association Molecular Dynamics Simulations. 2018 , 9, 2947	8
886	Best of Two Worlds? How MD Simulations of Amphiphilic Helical Peptides in Membranes Can Complement Data from Oriented Solid-State NMR. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 6002-6014	6.4 5
885	pH dependent membrane binding of the Solanum tuberosum plant specific insert: An in silico study. 2018 , 1860, 2608-2618	4
884	Interactions between the Molecular Components of the Cowpea Chlorotic Mottle Virus Investigated by Molecular Dynamics Simulations. 2018 , 122, 9490-9498	5
883	Molecular Dynamics Simulation of Protein Biosurfactants. 2018 , 2, 39	7
882	Insight into the Self-Assembling Properties of Peptergents: A Molecular Dynamics Simulation Study. 2018 , 19,	1
881	Peptide-Lipid Interaction Sites Affect Vesicles' Responses to Antimicrobial Peptides. 2018 , 115, 1518-1529	12

880	Reversible self-assembly of superstructured networks. 2018 , 362, 808-813	157
879	SNARE-mediated membrane fusion is a two-stage process driven by entropic forces. 2018 , 592, 3504-3515	7
878	Developing a Coarse-Grained Model for 1-Alkyl-3-methyl-imidazolium Chloride Ionic Liquids. 2018 , 57, 15206-15215	1
877	Theoretical Insights into the Interactions between Star-Shaped Antimicrobial Polypeptides and Bacterial Membranes. 2018 , 34, 13438-13448	11
876	A molecular dynamics approach towards evaluating osmotic and thermal stress in the extracellular environment. 2018 , 35, 559-567	6
875	TTClust: A Versatile Molecular Simulation Trajectory Clustering Program with Graphical Summaries. 2018 , 58, 2178-2182	48
874	Patchy Particle Model of the Hierarchical Self-Assembly of EConjugated Optoelectronic Peptides. 2018 , 122, 10219-10236	11
873	Folding and Lipid Composition Determine Membrane Interaction of the Disordered Protein COR15A. 2018 , 115, 968-980	14
872	Human Dystrophin Structural Changes upon Binding to Anionic Membrane Lipids. 2018 , 115, 1231-1239	6
871	Molecular details on the intermediate states of melittin action on a cell membrane. 2018 , 1860, 2234-2241	25
870	Molecular Dynamics Simulations of Kir2.2 Interactions with an Ensemble of Cholesterol Molecules. 2018 , 115, 1264-1280	32
869	A Martini coarse-grained model of the calcein fluorescent dye. 2018 , 51, 384002	6
868	Molecular simulation of the water-triolein-oleic acid mixture: Local structure and thermodynamic properties. 2018 , 148, 184702	8
867	Bibliography. 421-446	
866	An Amphipathic Helix Directs Cellular Membrane Curvature Sensing and Function of the BAR Domain Protein PICK1. 2018 , 23, 2056-2069	21
865	Coarse-Grained Molecular Dynamics Simulation of Sulerythrin and LARFH for Producing Protein Nanofibers. 2018 ,	
864	A Thermodynamic Funnel Drives Bacterial Lipopolysaccharide Transfer in the TLR4 Pathway. 2018 , 26, 1151-1161.e4	21
863	Molecular details of dimerization kinetics reveal negligible populations of transient μ -opioid receptor homodimers at physiological concentrations. 2018 , 8, 7705	26

862	Morphology and ion diffusion in PEDOT:Tos. A coarse grained molecular dynamics simulation. 2018 , 20, 17188-17198	43
861	Implicit-solvent dissipative particle dynamics force field based on a four-to-one coarse-grained mapping scheme. 2018 , 13, e0198049	6
860	Coarse-Grained Simulation of Protein-Imprinted Hydrogels. 2018 , 122, 7091-7101	9
859	The role of nanoparticle shape in translocation across the pulmonary surfactant layer revealed by molecular dynamics simulations. 2018 , 5, 1921-1932	17
858	Molecular Mechanism of Lipid Nanodisk Formation by Styrene-Maleic Acid Copolymers. 2018 , 115, 494-502	45
857	Molecular Perspective Mechanism for Drug Loading on Carbon Nanotube-Dendrimer: A Coarse-Grained Molecular Dynamics Study. 2018 , 122, 7956-7969	13
856	Elucidating Self-Assembling Peptide Aggregation via Morphoscanner: A New Tool for Protein-Peptide Structural Characterization. 2018 , 5, 1800471	4
855	Hybrid Particle-Field Molecular Dynamics Simulations of Charged Amphiphiles in an Aqueous Environment. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 4928-4937	6.4 13
854	Computational simulations for particles at interfaces. 2018 , 167-200	2
853	A polarizable MARTINI model for monovalent ions in aqueous solution. 2018 , 149, 163319	17
852	Simulation of Mixed Self-Assembled Monolayers on Gold: Effect of Terminal Alkyl Anchor Chain and Monolayer Composition. 2018 , 122, 7699-7710	9
851	Tailoring the Variational Implicit Solvent Method for New Challenges: Biomolecular Recognition and Assembly. 2018 , 5, 13	5
850	Roles of PIP2 in the membrane binding of MIM I-BAR: insights from molecular dynamics simulations. 2018 , 592, 2533-2542	8
849	How nanoscale protein interactions determine the mesoscale dynamic organisation of bacterial outer membrane proteins. 2018 , 9, 2846	33
848	Communication: Adaptive boundaries in multiscale simulations. 2018 , 148, 141104	8
847	Guiding principles for peptide nanotechnology through directed discovery. 2018 , 47, 3737-3758	79
846	Dimer Interface of the Human Serotonin Transporter and Effect of the Membrane Composition. 2018 , 8, 5080	22
845	Optimizing Protein-Polymer Interactions in a Poly(ethylene glycol) Coarse-Grained Model. 2018 , 122, 7997-8005	15

844	SNARE-mediated membrane fusion arrests at pore expansion to regulate the volume of an organelle. 2018 , 37,		24
843	Nanoparticles induced by embedding self-assembling cassette into glucagon-like peptide 1 for improving in vivo stability. 2018 , 32, 2992-3004		6
842	Learning Effective Molecular Models from Experimental Observables. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 3849-3858	6.4	26
841	Lipid-Protein Interactions Are Unique Fingerprints for Membrane Proteins. 2018 , 4, 709-717		139
840	A Funneled Conformational Landscape Governs Flavivirus Fusion Peptide Interaction with Lipid Membranes. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 3920-3932	6.4	6
839	Interactions of the EphA2 Kinase Domain with PIPs in Membranes: Implications for Receptor Function. 2018 , 26, 1025-1034.e2		20
838	Influence of pH on the activity of thrombin-derived antimicrobial peptides. 2018 , 1860, 2374-2384		19
837	Modeling the dynamics and kinetics of HIV-1 Gag during viral assembly. 2018 , 13, e0196133		8
836	A direct interaction of cholesterol with the dopamine transporter prevents its out-to-inward transition. 2018 , 14, e1005907		51
835	Molecular modeling of neurological membrane proteins - from binding sites to synapses. 2019 , 700, 38-49		2
834	Residue-Specialized Membrane Poration Kinetics of Melittin and Its Variants: Insight from Mechanistic Landscapes. 2019 , 71, 887		11
833	Coarse-graining molecular systems by spectral matching. 2019 , 151, 044116		17
832	Advances in protein structure prediction and design. 2019 , 20, 681-697		215
831	Recent Advances in Coarse-Grained Models for Biomolecules and Their Applications. 2019 , 20,		42
830	Physics-based oligomeric models of the yeast mitofusin Fzo1 at the molecular scale in the context of membrane docking. 2019 , 49, 234-244		8
829	A Simulation Study on the Interaction Between Pollutant Nanoparticles and the Pulmonary Surfactant Monolayer. 2019 , 20,		6
828	Whole-Cell Models and Simulations in Molecular Detail. 2019 , 35, 191-211		24
827	Mycolactone Toxin Membrane Permeation: Atomistic versus Coarse-Grained MARTINI Simulations. 2019 , 117, 87-98		9

826	Reconstitution reveals how myosin-VI self-organises to generate a dynamic mechanism of membrane sculpting. 2019 , 10, 3305	5
825	Permeation of beta-defensin-3 encapsulated with polyethylene glycol in lung surfactant models at air-water interface. 2019 , 182, 110357	8
824	Coarse-grained model of tropoelastin self-assembly into nascent fibrils. 2019 , 3, 100016	12
823	Implicit solvent systematic coarse-graining of dioleoylphosphatidylethanolamine lipids: From the inverted hexagonal to the bilayer structure. 2019 , 14, e0214673	3
822	A hybrid, bottom-up, structurally accurate, Go ² -like coarse-grained protein model. 2019 , 151, 044111	12
821	Membrane Recognition and Binding by the Phosphatidylinositol Phosphate Kinase PIP5K1A: A Multiscale Simulation Study. 2019 , 27, 1336-1346.e2	8
820	Aggregation kinetics of short peptides: All-atom and coarse-grained molecular dynamics study. 2019 , 253, 106219	3
819	Back-mapping based sampling: Coarse grained free energy landscapes as a guideline for atomistic exploration. 2019 , 151, 154102	8
818	Structural and functional insights into the tetrameric photosystem I from heterocyst-forming cyanobacteria. 2019 , 5, 1087-1097	31
817	Curvature induction and sensing of the F-BAR protein Pacsin1 on lipid membranes via molecular dynamics simulations. 2019 , 9, 14557	13
816	Structural basis for substrate specificity and regulation of nucleotide sugar transporters in the lipid bilayer. 2019 , 10, 4657	10
815	Serine Phosphorylation of L-Selectin Regulates ERM Binding, Clustering, and Monocyte Protrusion in Transendothelial Migration. 2019 , 10, 2227	2
814	A coarse-grained model for mechanical behavior of phosphorene sheets. 2019 , 21, 1884-1894	7
813	Ionic transport through a protein nanopore: a Coarse-Grained Molecular Dynamics Study. 2019 , 9, 15740	7
812	Magainin 2 and PGLa in Bacterial Membrane Mimics I: Peptide-Peptide and Lipid-Peptide Interactions. 2019 , 117, 1858-1869	18
811	Protein Allostery in Drug Discovery. 2019 ,	5
810	Ligand-Induced Conformational Dynamics of A Tyramine Receptor from <i>Sitophilus oryzae</i> . 2019 , 9, 16275	6
809	Resolution limit of data-driven coarse-grained models spanning chemical space. 2019 , 151, 164106	8

808	Computational Nanoscopy of Tight Junctions at the Blood-Brain Barrier Interface. 2019 , 20,		11
807	Influence of the long-range forces in non-Gaussian random-packing dynamics. 2019 , 383, 125884		3
806	Obtaining Protein Association Energy Landscape for Integral Membrane Proteins. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 6444-6455	6.4	6
805	MARTINI-Based Protein-DNA Coarse-Grained HADDOCKing. 2019 , 6, 102		12
804	Palmitoylation of Claudin-5 Proteins Influences Their Lipid Domain Affinity and Tight Junction Assembly at the Blood-Brain Barrier Interface. 2019 , 123, 983-993		13
803	A Practical View of the Martini Force Field. 2019 , 2022, 105-127		21
802	The structural basis of lipid scrambling and inactivation in the endoplasmic reticulum scramblase TMEM16K. 2019 , 10, 3956		55
801	Structural dataset from microsecond-long simulations of yeast mitofusin Fzo1 in the context of membrane docking. 2019 , 26, 104460		2
800	Insights into Membrane Protein-Lipid Interactions from Free Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 5727-5736	6.4	33
799	Surface Shear Viscosity and Interleaflet Friction from Nonequilibrium Simulations of Lipid Bilayers. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 6471-6481	6.4	9
798	Biophysical Insight on the Membrane Insertion of an Arginine-Rich Cell-Penetrating Peptide. 2019 , 20,		3
797	Less Is More: Coarse-Grained Integrative Modeling of Large Biomolecular Assemblies with HADDOCK. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 6358-6367	6.4	19
796	MARTINI-based simulation method for step-growth polymerization and its analysis by size exclusion characterization: a case study of cross-linked polyurethane. 2019 , 21, 21603-21614		8
795	Mining featured biomarkers associated with vascular invasion in HCC by bioinformatics analysis with TCGA RNA sequencing data. 2019 , 118, 109274		16
794	Peripheral Antimicrobial Peptide Gomesin Induces Membrane Protrusion, Folding, and Laceration. 2019 , 35, 13233-13242		3
793	Quantum Mechanical and Molecular Mechanics Modeling of Membrane-Embedded Rhodopsins. 2019 , 252, 425-449		5
792	Phospholipid Scramblases Remodel the Shape of Asymmetric Membranes. 2019 , 10, 6351-6354		5
791	Study of the Lamellar and Micellar Phases of Pluronic F127: A Molecular Dynamics Approach. 2019 , 7, 606		2

790	Understanding Interactions of Curcumin with Lipid Bilayers: A Coarse-Grained Molecular Dynamics Study. 2019 , 59, 4413-4426	6
789	Transferable coarse-grained MARTINI model for methacrylate-based copolymers. 2019 , 4, 186-198	5
788	Interactions between model inclusions on closed lipid bilayer membranes. 2019 , 40, 58-69	11
787	Modeling and Simulations of Polymers: A Roadmap. 2019 , 52, 755-786	161
786	Curvature-driven adsorption of cationic nanoparticles to phase boundaries in multicomponent lipid bilayers. 2019 , 11, 2767-2778	21
785	Top-down Multiscale Approach To Simulate Peptide Self-Assembly from Monomers. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 1514-1522	6.4 2
784	Ensemble Docking in Drug Discovery: How Many Protein Configurations from Molecular Dynamics Simulations are Needed To Reproduce Known Ligand Binding?. 2019 , 123, 5189-5195	42
783	Determining Critical Micelle Concentrations of Surfactants Based on Viscosity Calculations from Coarse-Grained Molecular Dynamics Simulations. 2019 , 33, 2408-2412	4
782	Role of Ligand Conformation on Nanoparticle-Protein Interactions. 2019 , 123, 1764-1769	13
781	Thermodynamically reversible paths of the first fusion intermediate reveal an important role for membrane anchors of fusion proteins. 2019 , 116, 2571-2576	32
780	Deciphering the Rules for Amino Acid Co-Assembly Based on Interlayer Distances. 2019 , 13, 1703-1712	12
779	CHARMM-GUI Nanodisc Builder for modeling and simulation of various nanodisc systems. 2019 , 40, 893-899	27
778	Curvature effect and stabilize ruptured membrane of BAX derived peptide studied by molecular dynamics simulations. 2019 , 88, 152-159	0
777	Tetrameric Charge-Zipper Assembly of the TisB Peptide in Membranes-Computer Simulation and Experiment. 2019 , 123, 1770-1779	2
776	Mechanisms of activity loss for a multi-PEGylated protein by experiment and simulation. 2019 , 12, 121-131	25
775	A coarse-grained multiscale model to simulate morphological changes of food-plant tissues undergoing drying. 2019 , 15, 901-916	8
774	Transmembrane domain dimerization induces cholesterol rafts in curved lipid bilayers. 2018 , 21, 268-274	5
773	A molecular dynamics study on the resilience of Sec61 channel from open to closed state.. 2019 , 9, 14876-14883	

772	Interaction of SNARE Mimetic Peptides with Lipid bilayers: Effects of Secondary Structure, Bilayer Composition and Lipid Anchoring. 2019 , 9, 7708	7
771	Membrane perforation by the pore-forming toxin pneumolysin. 2019 , 116, 13352-13357	49
770	Multiscale Modeling and Simulation Approaches to Lipid-Protein Interactions. 2019 , 2003, 1-30	4
769	Revealing a Dual Role of Ganglioside Lipids in the Aggregation of Membrane-Associated Islet Amyloid Polypeptide. 2019 , 252, 343-356	5
768	Atomistic Simulations of Membrane Ion Channel Conduction, Gating, and Modulation. 2019 , 119, 7737-7832	46
767	Self-Assembled Nanostructures of Peptide Amphiphiles: Charge Regulation by Size Regulation. 2019 , 123, 17606-17615	14
766	Pharmaceutical Nanotechnology. 2019 ,	3
765	Molecular-Level "Observations" of the Behavior of Gold Nanoparticles in Aqueous Solution and Interacting with a Lipid Bilayer Membrane. 2019 , 2000, 303-359	2
764	Exploring the impact of proteins on the line tension of a phase-separating ternary lipid mixture. 2019 , 150, 204702	5
763	Theoretical study on the stability of insulin within poly-isobutyl cyanoacrylate (PIBCA) nanocapsule. 2019 , 45, 896-903	1
762	Curvature induction and membrane remodeling by FAM134B reticulon homology domain assist selective ER-phagy. 2019 , 10, 2370	81
761	Resolving the conformational dynamics of ErbB growth factor receptor dimers. 2019 , 207, 225-233	6
760	Reduced level of docosahexaenoic acid shifts GPCR neuroreceptors to less ordered membrane regions. 2019 , 15, e1007033	11
759	Mechanistic insight into the early stages of amyloid formation using an anuran peptide. 2019 , 111, e24120	7
758	Revisiting the Meyer-Overton rule for drug-membrane permeabilities. 2019 , 117, 2900-2909	6
757	A non-conjugated polyethylenimine copolymer-based unorthodox nanoprobe for bioimaging and related mechanism exploration. 2019 , 7, 3016-3024	14
756	Multiscale modeling of material failure: Theory and computational methods. 2019 , 52, 1-103	22
755	Structural Investigation of Human Prolactin Receptor Transmembrane Domain Homodimerization in a Membrane Environment through Multiscale Simulations. 2019 , 123, 4858-4866	1

754	How Melittin Inserts into Cell Membrane: Conformational Changes, Inter-Peptide Cooperation, and Disturbance on the Membrane. 2019 , 24,	31
753	Structure and Dynamics of the Central Lipid Pool and Proteins of the Bacterial Holo-Translocon. 2019 , 116, 1931-1940	14
752	Coarse-graining involving virtual sites: Centers of symmetry coarse-graining. 2019 , 150, 154103	9
751	Simulating and analysing configurational landscapes of protein-protein contact formation. 2019 , 9, 20180062	9
750	Middle-way flexible docking: Pose prediction using mixed-resolution Monte Carlo in estrogen receptor β . 2019 , 14, e0215694	6
749	Biomimetic Lipid Membranes: Fundamentals, Applications, and Commercialization. 2019 ,	2
748	Dehydration-Driven Morphological Transformation of Flexible Vesicles on Liquid-Solid Interface. 2019 , 123, 12268-12275	
747	Molecular Dynamics Studies of Nanoparticle Transport Through Model Lipid Membranes. 2019 , 109-165	4
746	Machine Learning of Coarse-Grained Molecular Dynamics Force Fields. 2019 , 5, 755-767	160
745	A new method for the construction of coarse-grained models of large biomolecules from low-resolution cryo-electron microscopy data. 2019 , 21, 9720-9727	3
744	Multiconfigurational Coarse-Grained Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 3306-3315	6.4 13
743	Improved Intracellular Delivery of Polyarginine Peptides with Cargoes. 2019 , 123, 2636-2644	12
742	Enterovirus particles expel capsid pentamers to enable genome release. 2019 , 10, 1138	20
741	Binding of SV40's Viral Capsid Protein VP1 to Its Glycosphingolipid Receptor GM1 Induces Negative Membrane Curvature: A Molecular Dynamics Study. 2019 , 35, 3534-3544	4
740	Developing a Transferable Coarse-Grained Model for the Prediction of Thermodynamic, Structural, and Mechanical Properties of Polyimides at Different Thermodynamic State Points. 2019 , 59, 2009-2025	6
739	Coarse-Grained Simulation of Full-Length Integrin Activation. 2019 , 116, 1000-1010	9
738	ReaxFF MD Simulations of Peptide-Grafted Gold Nanoparticles. 2019 , 35, 5029-5036	11
737	Computational microscopy study of the granular structure and pH dependence of PEDOT:PSS. 2019 , 21, 6699-6711	27

736	Interaction of POPC, DPPC, and POPE with the β opioid receptor: A coarse-grained molecular dynamics study. 2019 , 14, e0213646		4
735	A Peptide-Nanoparticle System with Improved Efficacy against Multidrug Resistant Bacteria. 2019 , 9, 4485		57
734	Characterization of Lipid-Protein Interactions and Lipid-Mediated Modulation of Membrane Protein Function through Molecular Simulation. 2019 , 119, 6086-6161		80
733	Molecular Dynamics-Decorated Finite Element Method (MDeFEM): Application to the Gating Mechanism of Mechanosensitive Channels. 2019 , 77-128		
732	A Coarse-Grained Molecular Dynamics Approach to the Study of the Intrinsically Disordered Protein β Synuclein. 2019 , 59, 1458-1471		28
731	A Hybrid Hamiltonian for the Accelerated Sampling along Experimental Restraints. 2019 , 20,		5
730	The Devil Is in the Details: What Do We Really Track in Single-Particle Tracking Experiments of Diffusion in Biological Membranes?. 2019 , 10, 1005-1011		5
729	The SIRAH 2.0 Force Field: Altius, Fortius, Citius. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 2719-2733	6.4	53
728	Nanomediical Relevance of the Intermolecular Interaction Dynamics-Examples from Lysozymes and Insulins. 2019 , 4, 4206-4220		9
727	Parametrization of MARTINI for Modeling Hinging Motions in Membrane Proteins. 2019 , 123, 2254-2269		3
726	Developing and Testing of Lipid Force Fields with Applications to Modeling Cellular Membranes. 2019 , 119, 6227-6269		48
725	A lipid gating mechanism for the channel-forming O antigen ABC transporter. 2019 , 10, 824		34
724	Equations of motion for position-dependent coarse-grain mappings obtained with Mori-Zwanzig theory. 2019 , 150, 024108		4
723	Multiscale (re)modeling of lipid bilayer membranes. 2019 , 30, 39-104		1
722	Evaluating Models of Varying Complexity of Crowded Intrinsically Disordered Protein Solutions Against SAXS. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 6968-6983	6.4	10
721	Model reduction of rigid-body molecular dynamics via generalized multipole potentials. 2019 , 100, 063302		
720	Computational insights into lipid assisted peptide misfolding and aggregation in neurodegeneration. 2019 , 21, 22679-22694		9
719	The ABCG2 multidrug transporter is a pump gated by a valve and an extracellular lid. 2019 , 10, 5433		24

7 ¹⁸	Lipid Interactions of a Ciliary Membrane TRP Channel: Simulation and Structural Studies of Polycystin-2. 2020 , 28, 169-184.e5	22
7 ¹⁷	Large-scale, dynamin-like motions of the human guanylate binding protein 1 revealed by multi-resolution simulations. 2019 , 15, e1007193	6
7 ¹⁶	To Bud or Not to Bud: A Perspective on Molecular Simulations of Lipid Droplet Budding. 2019 , 6, 124	14
7 ¹⁵	19. Simulations of biological membranes with the Martini model. 2019 , 551-568	
7 ¹⁴	More Favorable Palmitic Acid Over Palmitoleic Acid Modification of Wnt3 Ensures Its Localization and Activity in Plasma Membrane Domains. 2019 , 7, 281	8
7 ¹³	Single-molecule studies of flavivirus envelope dynamics: Experiment and computation. 2019 , 143, 38-51	7
7 ¹²	Are the short cationic lipopeptides bacterial membrane disruptors? Structure-Activity Relationship and molecular dynamic evaluation. 2019 , 1861, 93-99	8
7 ¹¹	Helix-Switch Enables C99 Dimer Transition between the Multiple Conformations. 2019 , 59, 339-350	4
7 ¹⁰	Interplay between Membrane Curvature and Cholesterol: Role of Palmitoylated Caveolin-1. 2019 , 116, 69-78	33
7 ⁰⁹	State-dependent Lipid Interactions with the A2a Receptor Revealed by MD Simulations Using InVivo-Mimetic Membranes. 2019 , 27, 392-403.e3	42
7 ⁰⁸	Graph-Based Approach to Systematic Molecular Coarse-Graining. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 1199-1208	6.4 34
7 ⁰⁷	Coarse-graining Langevin dynamics using reduced-order techniques. 2019 , 380, 170-190	10
7 ⁰⁶	The lipid environment of Escherichia coli Aquaporin Z. 2019 , 1861, 431-440	19
7 ⁰⁵	Multiscale Modeling and Simulation of Nano-Carriers Delivery through Biological Barriers Review. 2019 , 2, 1800105	25
7 ⁰⁴	Martini coarse-grained model for polyethylenimine. 2019 , 40, 607-618	9
7 ⁰³	Lipid composition and salt concentration as regulatory factors of the anion selectivity of VDAC studied by coarse-grained molecular dynamics simulations. 2019 , 220, 66-76	3
7 ⁰²	Coarse-grained molecular dynamics of membrane semitoroidal pore formation in model lipid-peptide systems. 2019 , 87, 1-10	9
7 ⁰¹	The MemProtMD database: a resource for membrane-embedded protein structures and their lipid interactions. 2019 , 47, D390-D397	70

700	Conformational preferences and phase behavior of intrinsically disordered low complexity sequences: insights from multiscale simulations. 2019 , 56, 1-10		49
699	Mechanism of Enhanced Immature Dengue Virus Attachment to Endosomal Membrane Induced by prM Antibody. 2019 , 27, 253-267.e8		21
698	Modeling Lipid Membranes. 2019 , 741-759		
697	Cholesterol Interaction Sites on the Transmembrane Domain of the Hedgehog Signal Transducer and Class F G Protein-Coupled Receptor Smoothened. 2019 , 27, 549-559.e2		45
696	Multiscale modeling and simulations of protein adsorption: progresses and perspectives. 2019 , 41, 74-85		30
695	Computational Modeling of Realistic Cell Membranes. 2019 , 119, 6184-6226		265
694	Coarse-Grained Simulations of Peptide Nanoparticle Formation: Role of Local Structure and Nonbonded Interactions. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 1453-1462	6.4	8
693	A brief appraisal of computational modeling of antimicrobial peptides' activity. 2019 , 80, 28-32		6
692	Filling gaps in the knowledge of melittin on lipid membranes. 2019 , 561, 136-146		7
691	Modeling Interactions in Edible Fats. 2019 , 197-240		
690	Multiscale simulation of the interaction of calreticulin-thrombospondin-1 complex with a model membrane microdomain. 2019 , 37, 811-822		3
689	Membrane partitioning of peptide aggregates: coarse-grained molecular dynamics simulations. 2020 , 38, 524-532		1
688	Encapsulation of an endostatin peptide in liposomes: Stability, release, and cytotoxicity study. 2020 , 185, 110552		19
687	From directed evolution to computational enzyme engineering: a review. 2020 , 66, e16847		31
686	Interaction of naringin and naringenin with DPPC monolayer at the air-water interface. 2020 , 584, 124024		10
685	Multi-Peptide Adsorption on Uncharged Solid Surfaces: A Coarse-Grained Simulation Study. 2020 , 6, 186-195		3
684	Molecular dynamics study of membrane permeabilization by wild-type and mutant lytic peptides from the non-enveloped Flock House virus. 2020 , 1862, 183102		4
683	Biophysical characterization of the insertion of two potent antimicrobial peptides-Pin2 and its variant Pin2[GVG] in biological model membranes. 2020 , 1862, 183105		9

682	Computational simulations of TNF receptor oligomerization on plasma membrane. 2020 , 88, 698-709	4
681	Polymyxin B Loosens Lipopolysaccharide Bilayer but Stiffens Phospholipid Bilayer. 2020 , 118, 138-150	22
680	Determining Optimal Coarse-Grained Representation for Biomolecules Using Internal Cluster Validation Indexes. 2020 , 41, 14-20	4
679	An overview of data-driven HADDOCK strategies in CAPRI rounds 38-45. 2020 , 88, 1029-1036	6
678	Probing mechanical properties and failure mechanisms of fibrils of self-assembling peptides. 2020 , 2, 190-198	6
677	Molecular Dynamics of the Recruitment of Immunoreceptor Signaling Module DAP12 Homodimer to Lipid Raft Boundary Regulated by PIP2. 2020 , 124, 504-510	9
676	Assessing the effect of aromatic residue placement on the helical peptide structure and nanofibril formation of 21-mer peptides. 2020 , 5, 521-531	2
675	Magainin 2 and PGLa in Bacterial Membrane Mimics II: Membrane Fusion and Sponge Phase Formation. 2020 , 118, 612-623	15
674	Role of cholesterol-mediated effects in GPCR heterodimers. 2020 , 227, 104852	15
673	Machine learning for protein folding and dynamics. 2020 , 60, 77-84	55
672	Free Energies of the Disassembly of Viral Capsids from a Multiscale Molecular Simulation Approach. 2020 , 60, 974-981	13
671	Orientation Dependence of Inter-NCP Interaction: Insights into the Behavior of Liquid Crystal Phase and Chromatin Fiber Organization. 2020 , 124, 314-323	4
670	Development of Coarse-Grained Force Field by Combining Multilinear Interpolation Technique and Simplex Algorithm. 2020 , 41, 814-829	7
669	Structure of G-protein-coupled receptor heteromers. 2020 , 109-119	1
668	Cholesterol impacts chemokine CCR5 receptor ligand-binding activity. 2020 , 287, 2367-2385	5
667	A bipartite structural organization defines the SERINC family of HIV-1 restriction factors. 2020 , 27, 78-83	34
666	Computational reconstruction of atomistic protein structures from coarse-grained models. 2020 , 18, 162-176	24
665	Effect of membrane composition on DivIVA-membrane interaction. 2020 , 1862, 183144	1

664	A Comprehensive Study on Self-Assembly and Gelation of C-Dipeptides-From Design Strategies to Functionalities. 2020 , 21, 670-679	7
663	Engineering Chirally Blind Protein Pseudocapsids into Antibacterial Persisters. 2020 , 14, 1609-1622	26
662	Integrative Modelling of Biomolecular Complexes. 2020 , 432, 2861-2881	40
661	Subcellular localization of Rap1 GTPase activator CalDAG-GEFI is orchestrated by interaction of its atypical C1 domain with membrane phosphoinositides. 2020 , 18, 693-705	4
660	Martini Force Field for Protonated Polyethyleneimine. 2020 , 41, 349-361	4
659	pSPICA: A Coarse-Grained Force Field for Lipid Membranes Based on a Polar Water Model. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 782-793	6.4 8
658	Effect of concentration of PEG coated gold nanoparticle on lung surfactant studied with coarse-grained molecular dynamics simulations. 2020 , 266, 106457	0
657	Membrane targeting antimicrobial cyclic peptide nanotubes - an experimental and computational study. 2020 , 196, 111349	6
656	Exploring the Potential of Benzene-1,3,5-tricarboxamide Supramolecular Polymers as Biomaterials. 2020 , 21, 4105-4115	11
655	Comparison of umbrella sampling and steered molecular dynamics methods for computing free energy profiles of aromatic substrates through phospholipid bilayers. 2020 , 153, 034115	6
654	Learning Coarse-Grained Potentials for Binary Fluids. 2020 , 60, 3731-3745	0
653	PLD2-PI(4,5)P2 interactions in fluid phase membranes: Structural modeling and molecular dynamics simulations. 2020 , 15, e0236201	2
652	Extending the Martini Coarse-Grained Force Field to -Glycans. 2020 , 60, 3864-3883	7
651	Lecithin/isopropyl myristate reverse micelles as transdermal insulin carriers: Experimental evaluation and molecular dynamics simulation. 2020 , 59, 101891	3
650	Electric Field Induced Wetting of a Hydrophobic Gate in a Model Nanopore Based on the 5-HT Receptor Channel. 2020 , 14, 10480-10491	9
649	Titrateable Martini model for constant pH simulations. 2020 , 153, 024118	20
648	Insights into the mechanism of membrane fusion induced by the plant defense element, plant-specific insert. 2020 , 295, 14548-14562	3
647	Modeling Gas-Liquid Interfaces by Dissipative Particle Dynamics: Adsorption and Surface Tension of Cetyl Trimethyl Ammonium Bromide at the Air-Water Interface. 2020 , 36, 14686-14698	11

646	Coarse graining molecular dynamics with graph neural networks. 2020 , 153, 194101	34
645	Concentration- and pH-Dependent Oligomerization of the Thrombin-Derived C-Terminal Peptide TCP-25. 2020 , 10,	4
644	Integrative modeling of membrane-associated protein assemblies. 2020 , 11, 6210	9
643	Injectable Single-Component Peptide Depot: Autonomously Rechargeable Tumor Photosensitization for Repeated Photodynamic Therapy. 2020 , 14, 15793-15805	7
642	Triacylglycerols sequester monotopic membrane proteins to lipid droplets. 2020 , 11, 3944	13
641	Thermal Compaction of Disordered and Elastin-like Polypeptides: A Temperature-Dependent, Sequence-Specific Coarse-Grained Simulation Model. 2020 , 21, 3523-3538	5
640	ddcMD: A fully GPU-accelerated molecular dynamics program for the Martini force field. 2020 , 153, 045103	3
639	Versatile Dimerisation Process of Translocator Protein (TSPO) Revealed by an Extensive Sampling Based on a Coarse-Grained Dynamics Study. 2020 , 60, 3944-3957	3
638	A machine-learning-assisted study of the permeability of small drug-like molecules across lipid membranes. 2020 , 22, 19687-19696	7
637	Amyloidogenicity as a driving force for the formation of functional oligomers. 2020 , 212, 107604	2
636	MARTINI-Compatible Coarse-Grained Model for the Mesoscale Simulation of Peptoids. 2020 , 124, 7745-7764	10
635	Coarse-Grained Molecular Dynamics (CG-MD) Simulation of the Encapsulation of Dexamethasone in PSS/PDDA Layer-by-Layer Assembled Polyelectrolyte Nanocapsules. 2020 , 21, 292	3
634	Dynamin-2 R465W mutation induces long range perturbation in highly ordered oligomeric structures. 2020 , 10, 18151	1
633	Estimating the accuracy of the MARTINI model towards the investigation of peripheral protein-membrane interactions. 2021 ,	6
632	Assessing the Perturbing Effects of Drugs on Lipid Bilayers Using Gramicidin Channel-Based and Assays. 2020 , 63, 11809-11818	7
631	Impact of Cholesterol on the Stability of Monomeric and Dimeric Forms of the Translocator Protein TSPO: A Molecular Simulation Study. 2020 , 25,	4
630	The Effects of -Azidophenylalanine Incorporation on Protein Structure and Stability. 2020 , 60, 5117-5125	2
629	Functional Impact of the G279S Substitution in the Adenosine A1-Receptor (A1R-G279S7.44), a Mutation Associated with Parkinson's Disease. 2020 , 98, 250-266	1

628	BAK core dimers bind lipids and can be bridged by them. 2020 , 27, 1024-1031	23
627	Parametric Study of Lennard-Jones Potentials to Predict Physical Behavior via Coarse-Grained Molecular Dynamics Simulations of Water and Ethylene Glycol Over Wide Temporal and Spatial Scales. 2020 , 2, 153-160	
626	Aggregated Amphiphilic Antimicrobial Peptides Embedded in Bacterial Membranes. 2020 , 12, 44420-44432	14
625	Self-assembly and mesophase formation in a non-ionic chromonic liquid crystal: insights from bottom-up and top-down coarse-grained simulation models. 2020 , 16, 9488-9498	9
624	Predicting Small Molecule Transfer Free Energies by Combining Molecular Dynamics Simulations and Deep Learning. 2020 , 60, 5375-5381	13
623	Enzymatic Noncovalent Synthesis. 2020 , 120, 9994-10078	53
622	Closing the Gap Between Modeling and Experiments in the Self-Assembly of Biomolecules at Interfaces and in Solution. 2020 , 32, 8043-8059	4
621	Representation of the conformational ensemble of peptides in coarse grained simulations. 2020 , 153, 054108	
620	Evaluating inositol phospholipid interactions with inward rectifier potassium channels and characterising their role in disease. 2020 , 3,	8
619	The physicochemical properties role of a functionalized alkyl-peptide in nanofibre formation and neural progenitor cells viability and survival. 2020 , 91, 106829	
618	: Automatic Parametrization of Bonded Terms in MARTINI-Based Coarse-Grained Models of Simple to Complex Molecules Fuzzy Self-Tuning Particle Swarm Optimization. 2020 , 5, 32823-32843	11
617	The conformational and mutational landscape of the ubiquitin-like marker for autophagosome formation in cancer. 2021 , 17, 2818-2841	4
616	The Early Phase of β 2-Microglobulin Aggregation: Perspectives From Molecular Simulations. 2020 , 7, 578433	3
615	Quantitative Synaptic Biology: A Perspective on Techniques, Numbers and Expectations. 2020 , 21,	1
614	Quantum mechanics/molecular mechanics multiscale modeling of biomolecules. 2020 , 143-183	0
613	Protein Fibrils Formed by Rationally Designed β -Helical Peptides. 2020 , 36, 6126-6131	0
612	Coarse-grained (hybrid) integrative modeling of biomolecular interactions. 2020 , 18, 1182-1190	9
611	Interactions of a Bacterial RND Transporter with a Transmembrane Small Protein in a Lipid Environment. 2020 , 28, 625-634.e6	26

610	Sphingomyelin Effects in Caveolin-1 Mediated Membrane Curvature. 2020 , 124, 5177-5185	8
609	Coarse-Grained Force Field Calibration Based on Multiobjective Bayesian Optimization to Simulate Water Diffusion in Poly- β -caprolactone. 2020 , 124, 5042-5052	4
608	Chiral structure fluctuations predicted by a coarse-grained model of peptide aggregation. 2020 , 16, 5071-5080	1
607	Localization Preference of Antimicrobial Peptides on Liquid-Disordered Membrane Domains. 2020 , 8, 350	11
606	Capturing Protein-Ligand Recognition Pathways in Coarse-Grained Simulation. 2020 , 11, 5302-5311	10
605	CX3CL1 homo-oligomerization drives cell-to-cell adherence. 2020 , 10, 9069	5
604	The role of SP-B peptides in lung surfactant monolayers exposed to gold nanoparticles. 2020 , 22, 15231-152416	16
603	The Glycosphingolipid GM3 Modulates Conformational Dynamics of the Glucagon Receptor. 2020 , 119, 300-313	10
602	The acidic tail of HMGB1 regulates its secondary structure and conformational flexibility: A circular dichroism and molecular dynamics simulation study. 2020 , 18, 1160-1172	7
601	Cholesterol-mediated oligomerization pathways of serotonin G-coupled receptor 5-HT _{2C} . 2020 , 160, 1090-1100	3
600	Shuffled lipidation pattern and degree of lipidation determines the membrane interaction behavior of a linear cationic membrane-active peptide. 2020 , 578, 584-597	6
599	Effect of Protein Flexibility from Coarse-Grained Elastic Network Parameterizations on the Calculation of Free Energy Profiles of Ligand Binding. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 4734-4743	6.4 1
598	Differences and commonalities in plasma membrane recruitment of the two morphogenetically distinct retroviruses HIV-1 and MMTV. 2020 , 295, 8819-8833	2
597	Nanoscale Interplay of Membrane Composition and Amyloid Self-Assembly. 2020 , 124, 5837-5846	2
596	Capturing transient antibody conformations with DNA origami epitopes. 2020 , 11, 3114	26
595	Molecular Modeling and Simulations of Peptide-Polymer Conjugates. 2020 , 11, 257-276	17
594	Structure and Dynamics in the ATG8 Family From Experimental to Computational Techniques. 2020 , 8, 420	12
593	Discovery of Self-Assembling EConjugated Peptides by Active Learning-Directed Coarse-Grained Molecular Simulation. 2020 , 124, 3873-3891	37

592	Neighborhood Preference of Amino Acids in Protein Structures and its Applications in Protein Structure Assessment. 2020 , 10, 4371		2
591	Machine Learning Driven Analysis of Large Scale Simulations Reveals Conformational Characteristics of Ubiquitin Chains. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 3205-3220	6.4	5
590	Rotational Diffusion of Membrane Proteins in Crowded Membranes. 2020 , 124, 2994-3001		6
589	Coarse-grained MD simulations reveal beta-amyloid fibrils of various sizes bind to interfacial liquid-ordered and liquid-disordered regions in phase separated lipid rafts with diverse membrane-bound conformational states. 2020 , 260, 106355		12
588	Pulmonary Surfactant Lipid Reorganization Induced by the Adsorption of the Oligomeric Surfactant Protein B Complex. 2020 , 432, 3251-3268		17
587	On Calculating the Bending Modulus of Lipid Bilayer Membranes from Buckling Simulations. 2020 , 124, 6299-6311		18
586	Effect of Helical Kink on Peptide Translocation across Phospholipid Membranes. 2020 , 124, 5940-5947		5
585	Developing a Coarse-Grained Model for Bacterial Cell Walls: Evaluating Mechanical Properties and Free Energy Barriers. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 5369-5384	6.4	6
584	Functional Impact of the G279S Substitution in the Adenosine A-Receptor (AR-G279S), a Mutation Associated with Parkinson's Disease. 2020 , 98, 250-266		5
583	Data showing the lipid conformations and membrane binding behaviors of beta-amyloid fibrils in phase-separated cholesterol-enriched lipid domains with and without glycolipid and oxidized cholesterol from coarse-grained molecular dynamics simulations. 2020 , 30, 105496		1
582	Polymer-coated gold nanoparticles and polymeric nanoparticles as nanocarrier of the BP100 antimicrobial peptide through a lung surfactant model. 2020 , 314, 113661		6
581	Dynamic protein interfaces and conformational landscapes of membrane protein complexes. 2020 , 61, 191-197		17
580	Extension of the force-matching method to coarse-grained models with axially symmetric sites to produce transferable force fields: Application to the UNRES model of proteins. 2020 , 152, 054902		7
579	Capturing Choline-Aromatics Cation- π Interactions in the MARTINI Force Field. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 2550-2560	6.4	15
578	Physical properties of phospholipids and integral proteins and their biofunctional roles in pulmonary surfactant from molecular dynamics simulation.. 2020 , 10, 8568-8579		7
577	Not all therapeutic antibody isotypes are equal: the case of IgM IgG in Pertuzumab and Trastuzumab. 2020 , 11, 2843-2854		13
576	Charge-dependent interactions of monomeric and filamentous actin with lipid bilayers. 2020 , 117, 5861-5872		12
575	Characterizing Membrane Association and Periplasmic Transfer of Bacterial Lipoproteins through Molecular Dynamics Simulations. 2020 , 28, 475-487.e3		11

574	Order-disorder skewness in alpha-synuclein: a key mechanism to recognize membrane curvature. 2020 , 22, 5255-5263	7
573	Localized Axolemma Deformations Suggest Mechanoporation as Axonal Injury Trigger. 2020 , 11, 25	9
572	Multiple lipid binding sites determine the affinity of PH domains for phosphoinositide-containing membranes. 2020 , 6, eaay5736	17
571	Integrative Nanomedicine for New Therapies. 2020 ,	1
570	Computer simulations of protein-membrane systems. 2020 , 170, 273-403	15
569	Molecular dynamics trajectories for 630 coarse-grained drug-membrane permeations. 2020 , 7, 51	11
568	Structure and dynamics of liposomes designed for drug delivery: coarse-grained molecular dynamics simulations to reveal the role of lipopolymer incorporation.. 2020 , 10, 3745-3755	16
567	Development of transferable coarse-grained models of amino acids. 2020 , 5, 675-685	10
566	Extending the fused-sphere SAFT- Γ Mie force field parameterization approach to poly(vinyl butyral) copolymers. 2020 , 152, 044903	4
565	Different Anomeric Sugar Bound States of Maltose Binding Protein Resolved by a Cytolysin A Nanopore Tweezer. 2020 , 14, 1727-1737	12
564	Structural basis of proton-coupled potassium transport in the KUP family. 2020 , 11, 626	35
563	Lipid-dependent conformational landscape of the ErbB2 growth factor receptor dimers. 2020 , 230, 104911	2
562	The Effect of Force-Field Parameters on Cytochrome P450-Membrane Interactions: Structure and Dynamics. 2020 , 10, 7284	14
561	Membrane mediated toppling mechanism of the folate energy coupling factor transporter. 2020 , 11, 1763	8
560	Defining how multiple lipid species interact with inward rectifier potassium (Kir2) channels. 2020 , 117, 7803-7813	40
559	Membrane Thinning Induces Sorting of Lipids and the Amphipathic Lipid Packing Sensor (ALPS) Protein Motif. 2020 , 11, 250	7
558	Erratum: "Martini Coarse-Grained Model for Polyethylenimine" [J. Comput. Chem. 2019, 40, 607-618, DOI:10.1002/jcc.25747]. 2020 , 41, 1730-1734	1
557	Combining molecular dynamics simulations with small-angle X-ray and neutron scattering data to study multi-domain proteins in solution. 2020 , 16, e1007870	39

556	When Stiffness Matters: Mechanosensing in Heart Development and Disease. 2020 , 8, 334	28
555	MARTINI coarse-grained model for poly- ϵ -caprolactone in acetone-water mixtures. 2020 , 98, 1868-1879	4
554	Role of Cholesterol on Binding of Amyloid Fibrils to Lipid Bilayers. 2020 , 124, 3036-3042	8
553	Size-dependent aggregation of hydrophobic nanoparticles in lipid membranes. 2020 , 12, 9452-9461	5
552	Molecular dynamics simulations in photosynthesis. 2020 , 144, 273-295	25
551	Heterodimer and pore formation of magainin 2 and PGLa: The anchoring and tilting of peptides in lipid bilayers. 2020 , 1862, 183305	2
550	Molecular mechanism for bidirectional regulation of CD44 for lipid raft affiliation by palmitoylations and PIP2. 2020 , 16, e1007777	6
549	Arbitrary Resolution with Two Bead Types Coarse-Grained Strategy and Applications to Protein Recognition. 2020 , 11, 3263-3270	2
548	Computational modelling of flavivirus dynamics: The ins and outs. 2021 , 185, 28-38	2
547	Nanoparticles modified with cell penetrating peptides: Assessing adsorption on membranes containing acidic lipids. 2021 , 197, 111373	5
546	A review of advancements in coarse-grained molecular dynamics simulations. 2021 , 47, 786-803	30
545	Temperature dependent aggregation mechanism and pathway of lysozyme: By all atom and coarse grained molecular dynamics simulation. 2021 , 103, 107816	1
544	Multiscale molecular dynamics simulation study of polyoxyethylated alcohols self-assembly in emulsion systems. 2021 , 231, 116252	5
543	Dynamics of an LPS translocon induced by substrate and an antimicrobial peptide. 2021 , 17, 187-195	18
542	Elastic moduli of lipid membranes: Reproducibility of AFM measures. 2021 , 234, 105011	6
541	Self-assembling peptide hydrogels for the stabilization and sustained release of active Chondroitinase ABC in vitro and in spinal cord injuries. 2021 , 330, 1208-1219	16
540	Using coarse-grained models to examine structure-property relationships of diblock-arm star polymers. 2021 , 142, 110149	1
539	Using normal mode analysis on protein structural models. How far can we go on our predictions?. 2021 , 89, 531-543	3

538	Nanoscale modelling of polymer electrolytes for rechargeable batteries. 2021 , 36, 77-90		7
537	Structure and intermolecular interactions in spheroidal high-density lipoprotein subpopulations. 2021 , 5, 100042		0
536	Tailoring patchy nanoparticle design to modulate serum albumin adsorption and membrane interaction. 2021 , 17, 2071-2080		0
535	Simulation of FUS Protein Condensates with an Adapted Coarse-Grained Model. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 525-537	6.4	35
534	Structural Genomics. 2021 ,		1
533	Coarse-Grained Molecular Dynamics Simulations of Membrane Proteins: A Practical Guide. 2021 , 2302, 253-273		1
532	Lipid contact probability: an essential and predictive character for the structural and functional studies of membrane proteins.		1
531	Review: Simulation Models for Materials and Biomolecules. 2021 , 27-82		1
530	Nanocapsule designs for antimicrobial resistance. 2021 , 13, 10342-10355		4
529	Membrane Binding of Antimicrobial Peptides Is Modulated by Lipid Charge Modification. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 1218-1228	6.4	2
528	Using multiscale molecular dynamics simulations to obtain insights into pore forming toxin mechanisms. 2021 , 649, 461-502		4
527	Development of coarse-grained force field for alcohols: an efficient meta-multilinear interpolation parameterization algorithm. 2021 , 23, 1956-1966		2
526	Combining simulations and experiments for the molecular engineering of multifunctional collagen mimetic peptide-based materials. 2021 , 17, 1985-1998		5
525	Caveolin-1 and cavin1 act synergistically to generate a unique lipid environment in caveolae. 2021 , 220,		8
524	Coarse-Grained Force Fields from the Perspective of Statistical Mechanics: Better Understanding of the Origins of a MARTINI Hangover. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 1170-1180	6.4	10
523	3D Printing of Supramolecular Polymer Hydrogels with Hierarchical Structure. 2021 , 17, e2005743		24
522	Multiscale polarizable coarse-graining water models on cluster-level electrostatic dipoles. 2021 , 23, 8926-8935		2
521	The impact of Gag non-cleavage site mutations on HIV-1 viral fitness from integrative modelling and simulations. 2021 , 19, 330-342		4

520	Predicting the aptamer SYL3C-EpCAM complex's structure with the Martini-based simulation protocol. 2021 , 23, 7066-7079	2
519	Theoretical Aspects of XLPE-Based Blends and Nanocomposites. 2021 , 299-319	1
518	Capsid opening enables genome release of iflaviruses. 2021 , 7,	5
517	EnCurv: Simple Technique of Maintaining Global Membrane Curvature in Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 1181-1193	6.4 6
516	Membrane models for molecular simulations of peripheral membrane proteins. 2021 , 6, 1932589	0
515	Fentanyl binds to the μ opioid receptor via the lipid membrane and transmembrane helices.	2
514	Optimizing GEMARTINI Coarse-Grained Model for F-BAR Protein on Lipid Membrane. 2021 , 8, 619381	8
513	Molecular Dynamics Simulations of Ion-Containing Polymers Using Generic Coarse-Grained Models. 2021 , 54, 2031-2052	18
512	Interplay of folded domains and the disordered low-complexity domain in mediating hnRNPA1 phase separation. 2021 , 49, 2931-2945	26
511	Computational compound screening of biomolecules and soft materials by molecular simulations. 2021 , 29, 023001	8
510	Spontaneous Transmembrane Pore Formation by Short-chain Synthetic Peptide.	
509	Antibody cooperative adsorption onto AuNPs and its exploitation to force natural killer cells to kill HIV-infected T cells. 2021 , 36, 101056-101056	4
508	Effect of palmitoylation on the dimer formation of the human dopamine transporter. 2021 , 11, 4164	0
507	Molecular Dynamics Simulation of the n-Octacosane/Water Mixture Confined in Graphene Mesopores: Comparison of Atomistic and Coarse-Grained Calculations and the Effect of Catalyst Nanoparticle. 2021 , 35, 4313-4332	2
506	Selecting Collective Variables and Free-Energy Methods for Peptide Translocation across Membranes. 2021 , 61, 819-830	5
505	Molecular architecture of the endocytic TPLATE complex. 2021 , 7,	11
504	A multiscale simulation of amorphous polystyrene. 2021 , 28, 1	2
503	How the Strain Origin of Zika Virus NS1 Protein Impacts Its Dynamics and Implications to Their Differential Virulence. 2021 , 61, 1516-1530	7

502	Addressing the Excessive Aggregation of Membrane Proteins in the MARTINI Model. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 2513-2521	6.4	9
501	Perspectives on High-Throughput Ligand/Protein Docking With Martini MD Simulations. 2021 , 8, 657222		8
500	Hybrid resolution molecular dynamics simulations of amyloid proteins interacting with membranes. 2021 ,		1
499	Rotational dynamics of proteins in nanochannels: Role of solvent's local viscosity. 2021 ,		1
498	Full scale structural, mechanical and dynamical properties of HIV-1 liposomes.		
497	Identification and assessment of cardiolipin interactions with E. coli inner membrane proteins.		3
496	Assessing the Role of Calmodulin Linker Flexibility in Target Binding.		
495	CG2AT2: An Enhanced Fragment-based approach for Serial Multi-scale Molecular Dynamics simulations.		4
494	Membrane Interactions of β -Synuclein Revealed by Multiscale Molecular Dynamics Simulations, Markov State Models, and NMR. 2021 , 125, 2929-2941		1
493	Martini 3: a general purpose force field for coarse-grained molecular dynamics. 2021 , 18, 382-388		124
492	NMR structures and functional roles of two related chitin-binding domains of a lytic polysaccharide monooxygenase from <i>Cellvibrio japonicus</i> .		0
491	Bolaamphiphilic Bis-Dehydropeptide Hydrogels as Potential Drug Release Systems. 2021 , 7,		1
490	Surface science of cosmetic substrates, cleansing actives and formulations. 2021 , 290, 102383		8
489	Disease-linked TDP-43 hyperphosphorylation suppresses TDP-43 condensation and aggregation.		2
488	Thermodynamics and Free Energy Landscape of BAR-Domain Dimerization from Molecular Simulations. 2021 , 125, 3739-3751		1
487	HyperBeta: characterizing the structural dynamics of proteins and self-assembling peptides. 2021 , 11, 7783		
486	Cryo-EM Structures of CusA Reveal a Mechanism of Metal-Ion Export. 2021 , 12,		4
485	Multiscale Molecular Dynamics Studies Reveal Different Modes of Receptor Clustering by Gb3-Binding Lectins. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 2488-2501	6.4	4

484	TatA and TatB generate a hydrophobic mismatch that is important for function and assembly of the Tat translocon in Escherichia coli.	0
483	Refining conformational ensembles of flexible proteins against small-angle X-ray scattering data.	1
482	Ultra-coarse-graining of homopolymers in inhomogeneous systems. 2021 , 33,	3
481	Unusual mode of dimerization of retinitis pigmentosa-associated F220C rhodopsin. 2021 , 11, 10536	1
480	Molecular Dynamics Scoring of Protein-Peptide Models Derived from Coarse-Grained Docking. 2021 , 26,	2
479	Molecular Dynamics Simulations of Human Beta-Defensin Type 3 Crossing Different Lipid Bilayers. 2021 , 6, 13926-13939	3
478	Assessing the Role of Calmodulin's Linker Flexibility in Target Binding. 2021 , 22,	2
477	Deciphering ion transport and ATPase coupling in the intersubunit tunnel of KdpFABC.	
476	The Martini Model in Materials Science. 2021 , 33, e2008635	19
475	Investigating the Mechanism of Sodium Binding to SERT Using Direct Simulations. 2021 , 15, 673782	2
474	Conformational Reorganization of Apolipoprotein E Triggered by Phospholipid Assembly. 2021 , 125, 5285-5295	0
473	Enhanced translocation of amphiphilic peptides across membranes by transmembrane proteins. 2021 , 120, 2296-2305	1
472	Exploring the most stable aptamer/target molecule complex by the stochastic tunnelling-basin hopping-discrete molecular dynamics method. 2021 , 11, 11406	0
471	Molecular Insights into Pore Formation Mechanism, Membrane Perturbation, and Water Permeation by the Antimicrobial Peptide Pleurocidin: A Combined All-Atom and Coarse-Grained Molecular Dynamics Simulation Study. 2021 , 125, 7163-7176	2
470	Simulations of the Upper Critical Solution Temperature Behavior of Poly(ornithine--citrulline)s Using MARTINI-Based Coarse-Grained Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 4499-4511	6.4
469	Fast bilayer-micelle fusion mediated by hydrophobic dipeptides. 2021 , 120, 2330-2342	3
468	Interface Refinement of Low-to-Medium Resolution Cryo-EM Complexes using HADDOCK2.4.	
467	Dynamics and self-assembly of the SARS-CoV-2 spike transmembrane domain.	0

466	Modeling adsorption, conformation, and orientation of the Fis1 tail anchor at the mitochondrial outer membrane.	
465	From System Modeling to System Analysis: The Impact of Resolution Level and Resolution Distribution in the Computer-Aided Investigation of Biomolecules. 2021 , 8, 676976	8
464	Elucidating Axonal Injuries Through Molecular Modelling of Myelin Sheaths and Nodes of Ranvier. 2021 , 8, 669897	0
463	Neuropilin-1 assists SARS-CoV-2 infection by stimulating the separation of Spike protein S1 and S2. 2021 , 120, 2828-2837	19
462	Molecular Dynamics Simulations of Nanostructures Formed by Hydrophobins and Oil in Seawater. 2021 , 125, 7886-7899	0
461	Biomaterial interface with superior cell adhesive and antibacterial properties based on enzyme-triggered digestion of saliva acquired pellicle-inspired polypeptide coatings. 2021 , 415, 128955	7
460	PyLipID: A Python package for analysis of protein-lipid interactions from MD simulations.	3
459	Flexible pivoting of dynamin pleckstrin homology domain catalyzes fission: insights into molecular degrees of freedom. 2021 , 32, 1306-1319	1
458	In Silico Identification of Cholesterol Binding Motifs in the Chemokine Receptor CCR3. 2021 , 11,	3
457	Surface Properties of Nanoparticles Dictate Their Toxicity by Regulating Adsorption of Humic Acid Molecules.	7
456	Homo-oligomerization of the human adenosine A receptor is driven by the intrinsically disordered C-terminus. 2021 , 10,	5
455	Stability and Diffusion Properties of Insulin in Dissolvable Microneedles: A Multiscale Simulation Study. 2021 , 37, 9244-9252	0
454	Modulation of adenosine A2a receptor oligomerization by receptor activation and PIP interactions. 2021 , 29, 1312-1325.e3	2
453	Quantifying Membrane Curvature Sensing of Peripheral Proteins by Simulated Buckling and Umbrella Sampling. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 5276-5286	6.4 1
452	Diverse Aggregation Kinetics Predicted by a Coarse-Grained Peptide Model. 2021 , 125, 7587-7597	0
451	Retinyl esters form lipid droplets independently of triacylglycerol and seipin. 2021 , 220,	3
450	Aggregation of Lysozyme in the Presence of a Mixed Bilayer of POPC and POPG. 2021 , 6, 17861-17869	0
449	Inverse design of cholesterol attracting transmembrane helices reveals a paradoxical role of hydrophobic length.	0

448	Structural insights into the mechanism of human methyltransferase hPRMT4. 2021 , 1-14	
447	Simulation of A Bilayer Imitating the Inner Mitochondrial Membrane Using Coarse-Grained Molecular Dynamics. 2021 , 15, 652-654	
446	Anisotropic diffusion of membrane proteins at experimental timescales. 2021 , 155, 015102	1
445	PIP-induced membrane binding of the vinculin tail competes with its other binding partners. 2021 , 120, 4608-4622	1
444	Role of FAM134 paralogues in endoplasmic reticulum remodeling, ER-phagy, and Collagen quality control. 2021 , 22, e52289	10
443	Modeling of thermosensitive stereoregular polymers within the coarse-grained force field: Poly(N-isopropylacrylamide) as a benchmark case. 2021 , 33, 087110	0
442	Antimicrobial peptide induced colloidal transformations in bacteria-mimetic vesicles: Combining in silico tools and experimental methods. 2021 , 596, 352-363	5
441	Fusion pores with low conductance are cation selective. 2021 , 36, 109580	0
440	Identification and assessment of cardiolipin interactions with inner membrane proteins. 2021 , 7,	7
439	Molecular modeling prediction of albumin-based nanoparticles and experimental preparation, characterization, and in-vitro release kinetics of prednisolone from the nanoparticles. 2021 , 64, 102588	0
438	Microfluidic investigation of the effect of graphene oxide on mechanical properties of cell and actin cytoskeleton networks: experimental and theoretical approaches. 2021 , 11, 16216	3
437	A Generic Force Field for Simulating Native Protein Structures Using Dissipative Particle Dynamics.	
436	Deciphering ion transport and ATPase coupling in the intersubunit tunnel of KdpFABC. 2021 , 12, 5098	2
435	Interaction between the transmembrane domains of neurotrophin receptors p75 and TrkA mediates their reciprocal activation. 2021 , 297, 100926	2
434	An Association Test of the Spatial Distribution of Rare Missense Variants within Protein Structures Improves Statistical Power of Sequencing Studies.	
433	Coarse-Grained Modeling and Molecular Dynamics Simulations of Ca-Calmodulin. 2021 , 8, 661322	3
432	A Martini Coarse Grained Model of Citrate-Capped Gold Nanoparticles Interacting with Lipid Bilayers. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 6597-6609	6.4 2
431	Spontaneous transmembrane pore formation by short-chain synthetic peptide. 2021 , 120, 4557-4574	2

430	Modeling lipid-protein interactions for coarse-grained lipid and C α protein models. 2021 , 155, 155101	0
429	Theory and Practice of Coarse-Grained Molecular Dynamics of Biologically Important Systems. 2021 , 11,	6
428	Structure of the Shaker Kv channel and mechanism of slow C-type inactivation.	1
427	Structural variability and concerted motions of the T cell receptor - CD3 complex. 2021 , 10,	2
426	Evidence that specific interactions play a role in the cholesterol sensitivity of G protein-coupled receptors. 2021 , 1863, 183557	2
425	Dynamic assembly of the calcium hemostasis modulator 1 channel gates ATP permeation.	
424	The supramolecular organization of SARS-CoV and SARS-CoV-2 virions revealed by coarse-grained models of intact virus envelopes.	1
423	CG2AT2: an Enhanced Fragment-Based Approach for Serial Multi-scale Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 6472-6482	6.4 14
422	Structural and functional variation of chitin-binding domains of a lytic polysaccharide monoxygenase from <i>Cellvibrio japonicus</i> . 2021 , 297, 101084	2
421	Unveiling the structure of the primary caseinate particle using small-angle X-ray scattering and simulation methodologies. 2021 , 149, 110653	1
420	Scission energies of surfactant wormlike micelles loaded with nonpolar additives. 2021 , 604, 757-766	5
419	The nanotube express: Delivering a stapled peptide to the cell surface. 2021 , 604, 670-679	0
418	Macromolecular assembly and membrane activity of antimicrobial D,L- β -cyclic peptides. 2021 , 208, 112086	1
417	Enzyme self-aggregation in supramolecular self-assembly of glucose oxidase and catalase: Insight from molecular dynamics simulation based on coarse-grained method. 2022 , 552, 111366	1
416	Development of accurate coarse-grained force fields for weakly polar groups by an indirect parameterization strategy. 2021 , 23, 6763-6774	1
415	Dynamics of Human Serum Albumin Corona Formation on Gold Nanorods with Different Surface Ligands In Silico. 2021 , 125, 1181-1195	3
414	Seipin traps triacylglycerols to facilitate their nanoscale clustering in the endoplasmic reticulum membrane. 2021 , 19, e3000998	20
413	A generic force field for simulating native protein structures using dissipative particle dynamics. 2021 , 17, 9772-9785	2

412	Extension of the CAVS model to the simulation of helical peptides in a membrane environment. 2021 , 23, 12850-12863	0
411	Neuropilin-1 Assists SARS-CoV-2 Infection by Stimulating the Separation of Spike Protein Domains S1 and S2. 2021 ,	5
410	Identification and Characterization of Specific Protein-Lipid Interactions Using Molecular Simulation. 2021 , 2315, 121-139	2
409	Beneficent and Maleficent Effects of Cations on Bufadienolide Binding to Na,K-ATPase. 2021 , 61, 976-986	2
408	Coarse-Grained Parameterization of Nucleotide Cofactors and Metabolites: Protonation Constants, Partition Coefficients, and Model Topologies. 2021 , 61, 335-346	1
407	Protocol for Simulations of PEGylated Proteins with Martini 3. 2021 , 2199, 315-335	3
406	Coarse-Grained Models of Proteins: Theory and Applications. 2011 , 35-83	10
405	Lipid membranes for membrane proteins. 2015 , 1215, 73-90	2
404	Coarse-grained force fields for molecular simulations. 2015 , 1215, 125-49	15
403	In silico design of antimicrobial peptides. 2015 , 1268, 195-219	13
402	Molecular dynamics simulations of membrane proteins. 2013 , 1033, 85-101	19
401	Balancing bond, nonbond, and glike terms in coarse grain simulations of conformational dynamics. 2014 , 1084, 123-40	7
400	Molecular Dynamics Simulations in Drug Discovery and Drug Delivery. 2020 , 275-301	4
399	Modeling of Lipid Membranes and Lipoproteins. 2014 , 299-318	2
398	Chemosensorial G-proteins-coupled receptors: a perspective from computational methods. 2014 , 805, 441-57	4
397	Role of lipid-mediated effects in β adrenergic receptor dimerization. 2015 , 842, 247-61	19
396	Lipids in Regulation of the Mitochondrial Outer Membrane Permeability, Bioenergetics, and Metabolism. 2017 , 185-215	5
395	Modeling of Membrane Proteins. 2019 , 371-451	2

394	Molecular Dynamics Study of the Solution Behaviour of Antimicrobial Peptide Indolicidin. 2019 , 257-265	3
393	Coarse-grained molecular dynamics provides insight into the interactions of lipids and cholesterol with rhodopsin. 2014 , 796, 75-94	25
392	Advances in the Computational Identification of Allosteric Sites and Pathways in Proteins. 2019 , 1163, 141-169	12
391	Theoretical and computational advances in protein misfolding. 2019 , 118, 1-31	1
390	Coarse-grained molecular dynamics simulation of protein conformational change coupled to ligand binding. 2020 , 742, 137144	3
389	The dynamics of β -secretase and its substrates. 2020 , 105, 86-101	7
388	High-Resolution Insights into the Stepwise Self-Assembly of Nanofiber from Bioactive Peptides. 2017 , 121, 7421-7430	12
387	Chapter 1:Methods and Parameters for Membrane Simulations. 2010 , 1-25	3
386	Chapter 3:Coarse-grained Molecular Dynamics Simulations of Membrane Proteins. 2010 , 56-75	2
385	Molecular dynamics simulations reveal disruptive self-assembly in dynamic peptide libraries. 2017 , 15, 6541-6547	10
384	Predicting selectivity of paracellular pores for biomimetic applications. 2020 , 5, 686-696	2
383	Coarse-grained free-energy simulations of conformational state transitions in an adenosine 5'-triphosphate-binding cassette exporter. 2020 , 33, 712-716	1
382	Combining molecular dynamics simulations with small-angle X-ray and neutron scattering data to study multi-domain proteins in solution.	2
381	Dissecting the nanoscale lipid profile of caveolae.	1
380	Genetic, cellular and structural characterization of the membrane potential-dependent cell-penetrating peptide translocation pore.	2
379	Surface electrostatics govern the emulsion stability of biomolecular condensates.	12
378	Interplay of folded domains and the disordered low-complexity domain in mediating hnRNP A1 phase separation.	4
377	Modulation of A2aR Oligomerisation by Conformational State and PIP2 Interactions Revealed by MD Simulations and Markov Models.	3

376	The Impact of Gag Non-Cleavage Site Mutations on HIV-1 Viral Fitness from Integrative Modelling and Simulations.	2
375	The Automated Optimisation of a Coarse-Grained Force Field Using Free Energy Data.	2
374	Evaluating Inositol phospholipid interactions with Inward Rectifier Potassium Channels and characterising their role in Disease.	1
373	Simulation of FUS protein condensates with an adapted coarse-grained model.	1
372	Seipin traps triacylglycerols to facilitate their nanoscale clustering in the ER membrane.	2
371	State-Dependent Lipid Interactions with the A2a Receptor Revealed by MD Simulations Using In Vivo-Mimetic Membranes.	10
370	The structural basis of lipid scrambling and inactivation in the endoplasmic reticulum scramblase TMEM16K.	9
369	Insights into Membrane Protein-Lipid Interactions from Free Energy Calculations.	1
368	Less is more: Coarse-grained integrative modeling of large biomolecular assemblies with HADDOCK.	1
367	Lecithin:Retinol Acyl Transferase (LRAT) induces the formation of lipid droplets.	4
366	MARTINI bead form factors for the analysis of time-resolved X-ray scattering of proteins. 2014 , 47, 1190-1198	18
365	Ceramide chain length-dependent protein sorting into selective endoplasmic reticulum exit sites. 2020 , 6,	11
364	Coarse-Graining Parameterization and Multiscale Simulation of Hierarchical Systems. Part I. 2010 , 13-34	4
363	Lipid exchange mechanism of the cholesteryl ester transfer protein clarified by atomistic and coarse-grained simulations. 2012 , 8, e1002299	42
362	Closely related, yet unique: Distinct homo- and heterodimerization patterns of G protein coupled chemokine receptors and their fine-tuning by cholesterol. 2018 , 14, e1006062	24
361	High density lipoprotein structural changes and drug response in lipidomic profiles following the long-term fenofibrate therapy in the FIELD substudy. 2011 , 6, e23589	32
360	Line-tension controlled mechanism for influenza fusion. 2012 , 7, e38302	51
359	Aggregation of lipid-anchored full-length H-Ras in lipid bilayers: simulations with the MARTINI force field. 2013 , 8, e71018	33

358	Molecular dynamics simulation study of conformational changes of transcription factor TFIIIS during RNA polymerase II transcriptional arrest and reactivation. 2014 , 9, e97975	5
357	Formulation optimization and in vivo proof-of-concept study of thermosensitive liposomes balanced by phospholipid, elastin-like polypeptide, and cholesterol. 2014 , 9, e103116	17
356	Molecular dynamic simulation of the self-assembly of DAP12-NKG2C activating immunoreceptor complex. 2014 , 9, e105560	9
355	Dissipative Particle Dynamics Simulations for Phospholipid Membranes Based on a Four-To-One Coarse-Grained Mapping Scheme. 2016 , 11, e0154568	19
354	Excessive aggregation of membrane proteins in the Martini model. 2017 , 12, e0187936	89
353	Nanoengineering in biomedicine: Current development and future perspectives. 2020 , 9, 700-715	25
352	Recapturing the Correlated Motions of Protein Using Coarse- Grained Models. 2015 , 22, 654-9	2
351	Coarse-grained molecular dynamics simulations of biomolecules. 2014 , 1, 1-15	9
350	Interactions of Bio-Inspired Membranes with Peptides and Peptide-Mimetic Nanoparticles. 2015 , 2, 303-318	2
349	Simulation of lipid-protein interactions with the CgProt force field. 2017 , 4, 352-369	6
348	Theoretical and computational methods of protein liquid-liquid phase separation. 2020 , 69, 138701	1
347	The brown adipocyte protein CIDEA promotes lipid droplet fusion via a phosphatidic acid-binding amphipathic helix. 2015 , 4, e07485	72
346	Molecular basis for multimerization in the activation of the epidermal growth factor receptor. 2016 , 5,	91
345	v-SNARE transmembrane domains function as catalysts for vesicle fusion. 2016 , 5,	36
344	The hydrophobic nature of a novel membrane interface regulates the enzyme activity of a voltage-sensing phosphatase. 2018 , 7,	5
343	ATP-induced asymmetric pre-protein folding as a driver of protein translocation through the Sec machinery. 2019 , 8,	20
342	Effect of helical kink in antimicrobial peptides on membrane pore formation. 2020 , 9,	13
341	Large-scale state-dependent membrane remodeling by a transporter protein. 2019 , 8,	24

340	Structure of a mitochondrial ATP synthase with bound native cardiolipin. 2019 , 8,	36
339	Aromatic interactions with membrane modulate human BK channel activation. 2020 , 9,	1
338	Dynamic metastable long-living droplets formed by sticker-spacer proteins. 2020 , 9,	42
337	The automated optimisation of a coarse-grained force field using free energy data. 2021 , 23, 24842-24851	2
336	Physics-Based Coarse-Grained Modeling in Bio- and Nanochemistry. 2022 , 31-69	0
335	Improving the global dimensions of intrinsically disordered proteins in Martini 3.	1
334	Refining conformational ensembles of flexible proteins against small-angle x-ray scattering data. 2021 , 120, 5124-5135	5
333	Supramolecular Organization of Polymer Prodrug Nanoparticles Revealed by Coarse-Grained Simulations. 2021 , 143, 17412-17423	2
332	Mechanistic Understanding from Molecular Dynamics in Pharmaceutical Research 2: Lipid Membrane in Drug Design. 2021 , 14,	4
331	A Modeling-Based Design to Engineering Protein Hydrogels with Random Copolymers. 2021 , 15, 16139-16148	5
330	Mechanism of lipid droplet formation by the yeast Sei1/Ldb16 Seipin complex. 2021 , 12, 5892	5
329	Structure and Formation Mechanism of Antimicrobial Peptides Temporin B- and L-Induced Tubular Membrane Protrusion. 2021 , 22,	1
328	Visualization of complex processes in lipid systems using computer simulations and molecular graphics. 2009 , 580, 317-38	
327	Coarse-Graining Parameterization and Multiscale Simulation of Hierarchical Systems. Part II. 2010 , 35-68	
326	Computational Approaches and Simulation. 2012 , 213-263	
325	Modeling and Simulation of Hierarchical Protein Materials. 389-409	1
324	Software. 2013 , 403-429	
323	Towards a Coarse-Grained Model for Unfolded Proteins. 2013 , 3-10	0

- 322 Coarse-grained models of the proteins backbone conformational dynamics. **2014**, 805, 157-69 0
- 321 Bilayer Lipid Membrane Constructs: A Strategic Technology Evaluation Approach. 309-353 1
- 320 Coarse Grained Study of Amyloid Protofibril Aggregation. **2016**, 101-108
- 319 Modeling Lipid Membranes. **2016**, 1-19
- 318 MD Simulations of P-Type ATPases in a Lipid Bilayer System. **2016**, 1377, 459-92
- 317 A Physics-Based Coarse-Grained Model with Electric Multipoles. **2016**, 465-493
- 316 Lipid-Uptake Pathways and Lipid-Protein interactions in P-glycoprotein Revealed by Coarse-Grained Molecular Dynamics Simulations.
- 315 Molecular basis for the maintenance of lipid asymmetry in the outer membrane of *Escherichia coli*.
- 314 Specific cardiolipin-SecY interactions are required for proton-motive-force stimulation of protein secretion. 1
- 313 Interaction of lecithin-cholesterol acyltransferase with lipid surfaces and apolipoprotein A-I derived peptides: implications for the cofactor mechanism of apolipoprotein A-I.
- 312 Structural basis for endotoxin neutralization and anti-inflammatory activity of thrombin-derived C-terminal peptides.
- 311 Molecular Dynamics-Decorated Finite Element Method (MDeFEM): Application to the Gating Mechanism of Mechanosensitive Channels. **2018**, 1-52
- 310 Atomistic Simulation of Sol-Gel-Derived Hybrid Materials. **2018**, 1869-1902
- 309 Effects of Peptide Concentrations on Membrane Penetration from the Interaction of R9 Peptides with Asymmetric Lipid Bilayer. **2018**, 08, 16-25 0
- 308 Molecular Mechanics. 279-300
- 307 Cholesterol interaction sites on the transmembrane domain of the hedgehog signal transducer and Class F G protein-coupled receptor Smoothened.
- 306 Middle-way flexible docking: Pose prediction using mixed-resolution Monte Carlo in estrogen receptor β
- 305 Mechanism of Mycolactone Toxin Membrane Permeation: Atomistic vs Coarse-Grained MARTINI Simulations.

- 304 NEPRE: a Scoring Function for Protein Structures based on Neighbourhood Preference.
- 303 Flexible pivoting of dynamin PH-domain catalyzes fission: Insights into molecular degrees of freedom.
- 302 A β proton ratchet for coupling the membrane potential to protein transport. 0
- 301 Lipid Interactions of a Ciliary Membrane TRP Channel: Simulation and Structural Studies of Polycystin-2 (PC2). 1
- 300 Impact of pathogenic mutations of the GLUT1 glucose transporter on channel dynamics using ConsDYN enhanced sampling. 8, 322
- 299 Effect of Helical Kink in Antimicrobial Peptides on Membrane Pore Formation.
- 298 Magainin 2 and PGLa in Bacterial Membrane Mimics I: Peptide-Peptide and Lipid-Peptide Interactions. 0
- 297 Large-scale, dynamin-like motions of the human guanylate binding protein 1 revealed by multi-resolution simulations.
- 296 An overview of data-driven HADDOCK strategies in CAPRI rounds 38-45.
- 295 The structural basis for distinct binding avidity of Pertuzumab and Trastuzumab IgM towards HER2.
- 294 A ClyA nanopore tweezer for analysis of functional states of protein-ligand interactions. 1
- 293 Magainin 2 and PGLa in Bacterial Membrane Mimics II: Membrane Fusion and Sponge Phase Formation.
- 292 Localized axolemma deformations suggest mechanoporation as axonal injury trigger.
- 291 Interactions of a bacterial RND transporter with a transmembrane small protein in a lipid environment. 0
- 290 Liquid-liquid microphase separation leads to formation of membraneless organelles. 1
- 289 The CX3CL1 oligomerization is required for efficient CX3CR1-specific cell adherence.
- 288 Capturing Protein-Ligand Recognition Pathways in Coarse-grained Simulation.
- 287 Developing a Coarse-Grained Model for Bacterial Cell Walls and Evaluating Mechanical Properties and Free Energy Barriers.

- 286 Extending the Martini coarse-grained forcefield to N-glycans.
- 285 Electric Field Induced Wetting of a Hydrophobic Gate in a Model Nanopore Based on the 5-HT₃ Receptor Channel.
- 284 Structural Basis for Negative Regulation of ABA Signaling by ROP11 GTPase. 2
- 283 Membrane Interactions of β -Synuclein Revealed by Multiscale Molecular Dynamics Simulations, Markov State Models, and NMR.
- 282 Conformational Reorganisation of Apolipoprotein E Triggered by Phospholipid Assembly.
- 281 Molecular Simulations Guidelines for Biological Nanomaterials: From Peptides to Membranes. **2021**, 2208, 81-100
- 280 The TPLATE subunit is essential for structural assembly of the endocytic TSET complex. 0
- 279 Artificial intelligence reveals nuclear pore complexity. 7
- 278 Genetic, cellular, and structural characterization of the membrane potential-dependent cell-penetrating peptide translocation pore. **2021**, 10, 4
- 277 Oligomerization of the Human Adenosine A_{2A} Receptor is Driven by the Intrinsically Disordered C-terminus. 1
- 276 Unusual mode of dimerization of retinitis pigmentosa-associated F220C rhodopsin.
- 275 Thermodynamics and free energy landscape of BAR-domain dimerization from molecular simulations.
- 274 CHAPTER 3: Peptide Engineering Strategies. **2020**, 47-75
- 273 The Glycosphingolipid GM3 Modulates Conformational Dynamics of the Glucagon Receptor.
- 272 Modified Bacterial Lipids Which Alter Membrane Surface Charge Reduce Binding of Antimicrobial Peptides.
- 271 Integrative Modeling of Membrane-associated Protein Assemblies.
- 270 The guidance and adhesion protein FLRT2 dimerizes in cis via dual Small-X3-Small transmembrane motifs.
- 269 Beneficent and maleficent effects of cations on bufadienolide binding to Na⁺,K⁺-ATPase.

268	Fast Vesicle Fusion Mediated by Hydrophobic Dipeptides.	
267	Nanomaterials Interaction with Cell Membranes: Computer Simulation Studies. 2021 , 189-210	
266	Effects of Linker Flexibility and Conformational Changes of IP3 Receptor on Split Luciferase Complementation Assay. 2020 , 18, e2423	
265	The steroid mometasone alters protein containing lung surfactant monolayers in a concentration-dependent manner. 2021 , 111, 108084	1
264	Molecular simulation studies of self-assembly for a chromonic perylene dye: all-atom studies and new approaches to coarse-graining. 2021 , 118210	3
263	Editorial: Advanced Sampling and Modeling in Molecular Simulations for Slow and Large-Scale Biomolecular Dynamics. 2021 , 8, 795991	
262	Modeling the Structure, Dynamics, and Transformations of Proteins with the UNRES Force Field. 2022 , 2376, 399-416	0
261	Accurate Description of Protein-Protein Recognition and Protein Aggregation with the Implicit-Solvent-Based PACSAB Protein Model. 2021 , 13,	0
260	Nanocomposite of Fullerenes and Natural Rubbers: MARTINI Force Field Molecular Dynamics Simulations. 2021 , 13,	2
259	Molecular modeling of nanoplastic transformations in alveolar fluid and impacts on the lung surfactant film. 2021 , 127872	4
258	An Electrostatic-variable Coarse-grained Model for Predicting Enthalpy of Vaporization, Surface Tension, Diffusivity, Conductivity, and Dielectric Constant of Aqueous Ionic Liquid. 2021 , 346, 118230	0
257	A hybrid coarse-grained model for structure, solvation and assembly of lipid-like peptides.. 2021 ,	1
256	Multiscale simulations of protein and membrane systems.. 2021 , 72, 203-208	0
255	Gecko adhesion: a molecular-simulation perspective on the effect of humidity.. 2022 ,	4
254	Full scale structural, mechanical and dynamical properties of HIV-1 liposomes.. 2022 , 18, e1009781	0
253	Interpreting the Evolutionary Echoes of a Protein Complex Essential for Inner-Ear Mechanosensation.	
252	Occlusion of the human serotonin transporter is mediated by serotonin-induced conformational changes in the bundle domain.. 2022 , 101613	0
251	Surface Electrostatics Govern the Emulsion Stability of Biomolecular Condensates.. 2022 ,	7

250 Computational techniques to study protein dynamics and conformations. **2022**, 199-212

249 PyLipID: A Python Package for Analysis of Protein-Lipid Interactions from Molecular Dynamics Simulations.. *Journal of Chemical Theory and Computation*, **2022**, 6.4 10

248 Unraveling membrane properties at the organelle-level with LipidDyn.

247 Molecular Modeling for Reliability Issues. **2022**, 105-150

246 Molecular mechanisms of direct and indirect interplay between amyloid β 42 oligomer and characteristic lipids. **2022**,

245 Development of I Ion Channel Blockers Targeting Sulfonylurea Resistant Mutant K6.2 Based Channels for Treating DEND Syndrome.. **2021**, 12, 814066 1

244 Modeling Interactions within and between Peptide Amphiphile Supramolecular Filaments.. **2022**, 2

243 A Cholesterol Dimer Stabilizes the Inactivated State of an Inward-rectifier Potassium Channel.. **2022**, 2

242 Simulating Time-Resolved Dynamics of Biomolecular Systems. **2022**, 0

241 A Cholesterol Dimer Stabilizes the Inactivated State of an Inward-Rectifier Potassium Channel.

240 Sodium Binding Stabilizes the Outward-Open State of SERT by Limiting Bundle Domain Motions.. **2022**, 11, 1

239 Spontaneous Local Membrane Curvature Induced by Transmembrane Proteins.. **2022**, 1

238 Bak Core Dimer Focusses Triacylglycerides in the Membrane.. **2021**,

237 Disease-linked TDP-43 hyperphosphorylation suppresses TDP-43 condensation and aggregation.. **2022**, e108443 7

236 Toward an atomistic model of SARS-CoV-2. 1

235 Exploiting Endocytosis for Non-Spherical Nanoparticle Cellular Uptake. **2022**, 2, 1-16 2

234 Molecular simulation of linear octacosane a CG10 coarse grain scheme.. **2022**,

233 Evaluation of Interactions between SARS-CoV-2 RBD and Full-Length ACE2 with Coarse-Grained Molecular Dynamics Simulations.. **2022**, 1

232	Magainin 2 and PGLa in bacterial membrane mimics III: Membrane fusion and disruption.. 2022,	0
231	Conformational ensembles of intrinsically disordered proteins and flexible multidomain proteins.. 2022,	10
230	Peptide Self-assembly into stable Capsid-Like nanospheres and Co-assembly with DNA to produce smart artificial viruses.. 2022, 615, 395-407	2
229	Assessing the Stability of Biological Fibrils by Molecular-Scale Simulations.. 2022, 2340, 357-378	
228	Computational Models for the Study of Protein Aggregation.. 2022, 2340, 51-78	
227	Algorithms for protein design.. 2022, 130, 1-38	0
226	Data-driven discovery of cardiolipin-selective small molecules by computational active learning.	2
225	The Effect of Lipid Composition on the Dynamics of Tau Fibrils.	
224	An association test of the spatial distribution of rare missense variants within protein structures identify Alzheimer's disease-related patterns.. 2022,	1
223	Transition between conformational states of the TREK-1 K2P channel promoted by interaction with PIP2.	
222	Salt Destabilization of Cationic Colistin Complexation within Polyanionic Microgels. 2022, 55, 1736-1746	1
221	Specific interactions of peripheral membrane proteins with lipids: what can molecular simulations show us?. 2022,	2
220	Replenishing HDL with synthetic HDL has multiple protective effects against sepsis in mice.. 2022, 15, eabl9322	0
219	Mechanistic Pathway of Lipid Phase-Dependent Lipid Corona Formation on Phenylalanine-Functionalized Gold Nanoparticles: A Combined Experimental and Molecular Dynamics Simulation Study.. 2022, 126, 2241-2255	2
218	Ligand-independent oligomerization of TACI is controlled by the transmembrane domain and regulates proliferation of activated B cells.. 2022, 38, 110583	0
217	Interaction With the Lipid Membrane Influences Fentanyl Pharmacology. 2,	1
216	mPPases create a conserved anionic membrane fingerprint as identified via multi-scale simulations.	
215	Standard Binding Free Energy and Membrane Desorption Mechanism for a Phospholipase C.. 2022,	1

214	Efficient quantification of lipid packing defect sensing by amphipathic peptides; comparing Martini 2 & 3 with CHARMM36.		
213	Large Scale Hydrodynamically Coupled Brownian Dynamics Simulations of Polymer Solutions Flowing through Porous Media.. 2022 , 14,		0
212	Membrane contact probability: An essential and predictive character for the structural and functional studies of membrane proteins.. 2022 , 18, e1009972		1
211	Cryo-EM structure of the heptameric calcium homeostasis modulator 1 channel.. 2022 , 101838		0
210	A molecular switch controls the impact of cholesterol on a Kir channel.. 2022 , 119, e2109431119		3
209	Computational models for studying physical instabilities in high concentration biotherapeutic formulations.. 2022 , 14, 2044744		1
208	Voltage-Induced Adsorption of Cationic Nanoparticles on Lipid Membranes.. 2022 ,		0
207	Membrane interactions of mitochondrial lipid transfer proteins.		1
206	Interface refinement of low- to medium-resolution Cryo-EM complexes using HADDOCK2.4.. 2022 ,		1
205	Improving Martini 3 for Disordered and Multidomain Proteins.. <i>Journal of Chemical Theory and Computation</i> , 2022 ,	6.4	5
204	Polypeptide coatings on biominerals with superior antimicrobial and antifouling properties inspired by human salivary proteins. 2022 , 27, 101446		
203	Coarse-Grain Simulations of Membrane-Adsorbed Helical Peptides.. 2022 , 2405, 137-150		
202	. 2021 ,		1
201	Supramolecular Organization of SARS-CoV and SARS-CoV-2 Virions Revealed by Coarse-Grained Models of Intact Virus Envelopes.. 2021 ,		3
200	pH-dependent behavior of ionizable cationic lipids in mRNA-carrying lipoplexes investigated by molecular dynamics simulations. 2021 , e2100683		1
199	Assembly and Analysis of Cell-Scale Membrane Envelopes.. 2021 ,		2
198	Structural, functional and computational studies of membrane recognition by Plasmodium Perforin-Like Proteins 1 and 2.		
197	Competitive and/or cooperative interactions of graphene-family materials and benzo[a]pyrene with pulmonary surfactant: a computational and experimental study.. 2021 , 18, 46		0

196 Effects of Cholesterol on the mechanism of fengycin, a biofungicide.. **2022,**

195 Molecular Dynamics Simulation Studies on the Aggregation of Amyloid- β Peptides and Their Disaggregation by Ultrasonic Wave and Infrared Laser Irradiation.. **2022, 27,**

0

194 Distinct lipid membrane interaction and uptake of differentially charged nanoplastics in bacteria.. **2022, 20, 191**

1

193 Chapter 7. Molecular Modelling of Nucleic Acids. 165-197

192 Table_1.docx. **2019,**

191 Video_1.mp4. **2019,**

190 Video_2.mp4. **2019,**

189 Video_3.mp4. **2019,**

188 Video_4.mp4. **2019,**

187 Data_Sheet_1.pdf. **2018,**

186 Data_Sheet_1.PDF. **2020,**

185 Data_Sheet_2.zip. **2020,**

184 Data_Sheet_1.PDF. **2019,**

183 Data_Sheet_1.XLSX. **2020,**

182 Table_1.DOCX. **2020,**

181 Data_Sheet_1.PDF. **2020,**

180 Video_1.mpeg. **2020,**

179 Video_2.mpeg. **2020,**

178 Data_Sheet_1.PDF. 2020,

177 Video_1.mp4. 2020,

176 Video_2.mp4. 2020,

175 Video_3.mp4. 2020,

174 Video_4.mp4. 2020,

173 Video_5.mp4. 2020,

172 Molecular Mechanisms Underlying Caveolin-1 Mediated Membrane Curvature.. 2022, 1

0

171 Structure of the Shaker Kv channel and mechanism of slow C-type inactivation.. 2022, 8, eabm7814

7

170 Rate-limiting transport of positively charged arginine residues through the Sec-machinery is integral to the mechanism of protein secretion.. 2022, 11,

1

169 Dimerization of the pulmonary surfactant protein C in a membrane environment.. 2022, 17, e0267155

1

168 Multiscale MD simulations of wild-type and sickle hemoglobin aggregation.. 2022,

167 Nanopore Sensing Technique for Studying the Hofmeister Effect.. 2022, e2200921

0

166 Structure of C. elegans TMC-1 complex illuminates auditory mechanosensory transduction.

1

165 Adsorption of Pulmonary and Exogeneous Surfactants on SARS-CoV-2 Spike Protein.. 2022,

164 Mechanism behind Polysorbates' Inhibitory Effect on P-Glycoprotein.. 2022,

0

163 Development of a Hybrid-Resolution Force Field for Peptide Self-Assembly Simulations: Optimizing Peptide-Peptide and Peptide-Solvent Interactions.. 2022,

2

162 The Val34Met, Thr164Ile and Ser220Cys Polymorphisms of the β 2-Adrenergic Receptor and Their Consequences on the Receptor Conformational Features: A Molecular Dynamics Simulation Study. 2022, 23, 5449

161 Investigation of the structural and dynamical properties of human uncoupling protein 2 through molecular dynamics simulations.. 2022, 114, 108203

160	Structural dynamics of smoothened (SMO) in the ciliary membrane and its interaction with membrane lipids.. 2022 , 183946		0
159	Cooperative antimicrobial action of melittin on lipid membranes: A coarse-grained molecular dynamics study.. 2022 , 1864, 183955		0
158	Seipin transmembrane segments critically function in triglyceride nucleation and lipid droplet budding from the membrane.. 2022 , 11,		1
157	Structural Bases for the Involvement of Phosphatidylinositol-4,5-bisphosphate in the Internalization of the Cell-Penetrating Peptide Penetratin.		0
156	Molecular Modeling of Nanoparticles. 2022 , 681-703		
155	Transition between conformational states of the TREK-1 K2P channel promoted by interaction with PIP2. 2022 ,		0
154	Structural, Functional and Computational Studies of Membrane Recognition by Plasmodium Perforin-Like Proteins 1 and 2. 2022 , 434, 167642		
153	Molecular basis of transport of surface functionalised gold nanoparticles to pulmonary surfactant. 2022 , 12, 18012-18021		
152	Peptide mediated colorimetric detection of SARS-CoV-2 using gold nanoparticles: a molecular dynamics simulation study. 2022 , 28,		
151	Two decades of Martini: Better beads, broader scope.		5
150	Discovering Novel Small Molecule Compound for Prevention of Monoclonal Antibody Self-Association. 2022 , 11, 40		0
149	Efficient Quantification of Lipid Packing Defect Sensing by Amphipathic Peptides: Comparing Martini 2 and 3 with CHARMM36. <i>Journal of Chemical Theory and Computation</i> ,	6.4	2
148	Automated Protein Secondary Structure Assignment from C α Positions Using Neural Networks. 2022 , 12, 841		
147	Extracting time series matching a small-angle X-ray scattering profile from trajectories of molecular dynamics simulations. 2022 , 12,		
146	Impact of Surface Polarity on Lipid Assembly under Spatial Confinement. 2022 , 38, 7545-7557		
145	Impact of pathogenic mutations of the GLUT1 glucose transporter on solute carrier dynamics using ComDYN enhanced sampling. 8, 322		
144	Molecular Mechanism of CD44 Homodimerization Modulated by Palmitoylation and Membrane Environments. 2022 ,		
143	Interactions on Proteins Arising from the Self-Assembly of a Polyelectrolyte Brush.		

142	Pore Formation Mechanism of A-Beta Peptide on the Fluid Membrane: A Combined Coarse-Grained and All-Atomic Model. 2022 , 27, 3924		
141	Key aspects of the past 30 Years of protein design.		1
140	The guidance and adhesion protein FLRT2 dimerizes in cis via dual small-X3-small transmembrane motifs. 2022 ,		0
139	AI-based structure prediction empowers integrative structural analysis of human nuclear pores. 2022 , 376,		10
138	Simulation study of domain formation in a model bacterial membrane.		0
137	Unraveling membrane properties at the organelle-level with LipidDyn. 2022 , 20, 3604-3614		1
136	PolyethylenimineDNA Nanoparticles under Endosomal Acidification and Implication to Gene Delivery. 2022 , 38, 8382-8397		1
135	Molecular dynamics simulations of ovalbumin adsorption at squalene/water interface. 2022 ,		
134	Antibodynanobody combination increases their neutralizing activity against SARS-CoV-2 and nanobody H11-H4 is effective against Alpha, Kappa and Delta variants. 2022 , 12,		1
133	TatA and TatB generate a hydrophobic mismatch important for the function and assembly of the Tat translocon in Escherichia coli. 2022 , 102236		0
132	Multifaceted Computational Modeling in Glycoscience.		7
131	Accurate and Efficient Estimation of Lennard-Jones Interactions for Coarse-Grained Particles via a Potential Matching Method. <i>Journal of Chemical Theory and Computation</i> ,	6.4	0
130	In Silico Assessment of the Lipid Fingerprint Signature of ATP2, the Essential P4-ATPase of Malaria Parasites. 2022 , 12, 702		
129	Implementation of Telescoping Boxes in Adaptive Steered Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> ,	6.4	0
128	Computational and Experimental Evaluation of the Stability of a GLP-1-like Peptide in EthanolWater Mixtures. 2022 , 14, 1462		
127	Coarse-Grained Water Model Development for Accurate Dynamics and Structure Prediction.		
126	Effect of Cholesterol on C99 Dimerization: Revealed by Molecular Dynamics Simulations. 9,		1
125	Cardiolipin, and not monolysocardiolipin, preferentially binds to the interface of Complexes III and IV.		

124	Asynchronous Reciprocal Coupling of Martini 2.2 Coarse-Grained and CHARMM36 All-Atom Simulations in an Automated Multiscale Framework. <i>Journal of Chemical Theory and Computation</i> , 6.4	0
123	Effect of temperature, pH, and terminal groups on structural properties of carbon nanotube-dendrimer composites: A coarse-grained molecular dynamics simulation study. 2022 , 363, 119825	0
122	A Theoretical Perspective on the Thermodynamic Stability of Polymer Blends for Solar Cells: From Experiments to Predictive Modeling. 2200172	2
121	Modeling Adsorption, Conformation, and Orientation of the Fis1 Tail Anchor at the Mitochondrial Outer Membrane. 2022 , 12, 752	
120	Transferable and Polarizable Coarse Grained Model for Proteins-ProMPT. 2022 , 18, 5046-5055	2
119	Polymyxins induce lipid scrambling and disrupt the homeostasis of Gram-negative bacteria membrane. 2022 ,	0
118	Side Chain Geometry Determines the Fibrillation Propensity of a Minimal Two-Beads-per-Residue Peptide Model. 2022 , 126, 5772-5780	
117	Facilitating CG simulations with MAD: the MArtini Database Server.	0
116	Concentration-dependent cortisone adsorption and interaction with model lung surfactant monolayer. 1-12	1
115	Nucleation and growth of gold nanoparticles in the presence of different surfactants. A dissipative particle dynamics study. 2022 , 12,	0
114	Exploring the binding kinetics and behaviors of self-aggregated beta-amyloid oligomers to phase-separated lipid rafts with or without ganglioside-clusters. 2022 , 106874	0
113	ABCA1 is an extracellular phospholipid translocase. 2022 , 13,	1
112	The effect of lipid composition on the dynamics of tau fibrils.	1
111	COGRIMEN: Coarse-Grained Method for Modeling of Membrane Proteins in Implicit Environments.	
110	The effects of serum albumin pre-adsorption of nanoparticles on protein corona and membrane interaction: A molecular simulation study. 2022 , 167771	0
109	Antifouling performance and mechanism analysis of marine peptide modified aluminum alloy surface. 2022 , 445, 128742	0
108	Protocol to study the oligomeric organization of single-span transmembrane peptides using molecular dynamics simulations. 2022 , 3, 101636	
107	Anionic lipids induce a fold-unfold transition in the membrane-translocating Engrailed homeodomain. 2022 , 1864, 184030	

106	Nanoporous Membranes of Densely Packed Carbon Nanotubes Formed by Lipid-Mediated Self-Assembly.	0
105	Structural basis for membrane attack complex inhibition by CD59.	0
104	SARS-CoV -2 spike protein aggregation is triggered by bacterial lipopolysaccharide.	0
103	Transposition of polymer-encapsulated small interfering RNA through lung surfactant models at the air-water interface. 2022 , 563, 111704	0
102	Theoretical study of macrocyclic host molecules: from supramolecular recognition to self-assembly. 2022 , 24, 19011-19028	1
101	Computational design of self-assembling peptide chassis materials for synthetic cells.	0
100	Performance efficient macromolecular mechanics via sub-nanometer shape based coarse graining.	1
99	Lipid Modulation of a Class B GPCR: Elucidating the Modulatory Role of PI(4,5)P2 Lipids.	2
98	Deep inside molecules - digital twins at the nanoscale. 2022 , 4, 324-341	0
97	Antimicrobial Peptide Mechanism Studied by Scattering-Guided Molecular Dynamics Simulation. 2022 , 126, 6922-6935	0
96	The dynamic interplay of PIP 2 and ATP in the regulation of the K ATP channel.	1
95	Comparative Study of State-Dependent Cholesterol Binding Sites in Adenosine A2A and A1 Receptors Using Coarse-Grained Molecular Dynamics Simulations in Biologically Relevant Membranes.	0
94	Unique structural features of claudin-5 and claudin-15 lead to functionally distinct tight junction strand architecture.	0
93	Toward Accurate Coarse-Grained Simulations of Disordered Proteins and Their Dynamic Interactions. 2022 , 62, 4523-4536	1
92	Computer-Aided Design of Lasso-like Self-Assembling Anticancer Peptides with Multiple Functions for Targeted Self-Delivery and Cancer Treatments. 2022 , 16, 13783-13799	0
91	A coarse-grained approach to NMR -data-assisted modeling of protein structures.	0
90	The NALCN channel regulates metastasis and nonmalignant cell dissemination.	1
89	Insight into the Initial Stages of the Folding Process in Onconase Revealed by UNRES.	0

88	Zwitterionic Biomaterials.	6
87	Cofilin-Membrane Interactions: Electrostatic Effects in Phosphoinositide Lipid Binding.	0
86	Organizations of melittin peptides after spontaneous penetration into cell membranes. 2022 ,	0
85	mPPases create a conserved anionic membrane fingerprint as identified via multi-scale simulations. 2022 , 18, e1010578	0
84	Computational tools to study RNA-protein complexes. 9,	0
83	Modeling of supramolecular biopolymers: Leading the in silico revolution of tissue engineering and nanomedicine. 2022 , 11, 2965-2996	0
82	Cardiolipin, and not monolysocardiolipin, preferentially binds to the interface of Complexes III and IV.	0
81	No dance, no partner! A tale of receptor flexibility in docking and virtual screening. 2022 ,	0
80	Self-assembly of an in silico designed dipeptide derivative to obtain photo-responsive vesicles.	0
79	Multiscale modelling of claudin-based assemblies: a magnifying glass for novel structures of biological interfaces. 2022 ,	0
78	Towards design of drugs and delivery systems with the Martini coarse-grained model. 1-51	1
77	Mitochondrial phospholipid import mediated by VDAC, a dimeric beta barrel scramblase.	0
76	How Does Gecko Keratin Stick to Hydrophilic and Hydrophobic Surfaces in the Presence and Absence of Water? An Atomistic Molecular Dynamics Investigation.	1
75	Adaptive force biasing algorithms: New convergence results and tensor approximations of the bias. 2022 , 32,	0
74	Effective Molecular Dynamics from Neural-Network Based Structure Prediction Models.	0
73	Machine learning overcomes human bias in the discovery of self-assembling peptides.	3
72	Magainin 2 and PGLa in Bacterial Membrane Mimics IV: Membrane Curvature and Partitioning. 2022 ,	0
71	Self-Defensive Antimicrobial Surfaces Using Polymyxin-Loaded Poly(styrene sulfonate) Microgels.	1

70	Hierarchical Materials from High Information Content Macromolecular Building Blocks: Construction, Dynamic Interventions, and Prediction.	2
69	Structures of the TMC-1 complex illuminate mechanosensory transduction. 2022 , 610, 796-803	2
68	Designed Complex Peptide-based Adaptive Systems: A Bottom-up Approach.	0
67	Synergistic and Competitive Lipid Interactions in the Serotonin1A Receptor Microenvironment.	1
66	Atomistic Pictures of Self-Assembled Helical Peptide Nanofibers.	0
65	Exploring Membrane Binding Targets of Disordered Human Tau Aggregates on Lipid Rafts Using Multiscale Molecular Dynamics Simulations. 2022 , 12, 1098	1
64	Optimizing the Martini 3 force field reveals the effects of the intricate balance between protein-water interaction strength and salt concentration on biomolecular condensate formation.	0
63	Predictive Molecular Models for Charged Materials Systems: From Energy Materials to Biomacromolecules. 2204272	0
62	Febrile temperatures modulate the formation of immune complexes relevant for autoimmune diseases. 2023 , 111, 103425	0
61	Identification of possible binding modes of SARS-CoV-2 spike N-terminal domain for ganglioside GM1. 2023 , 812, 140260	0
60	Multiscale Computational Approaches toward the Understanding of Materials. 2200628	1
59	Lipid bicelles in the study of biomembrane characteristics.	0
58	Mutational Insight into Allosteric Regulation of Kir Channel Activity. 2022 , 7, 43621-43634	0
57	Hierarchical Coarse-Grained Strategy for Macromolecular Self-Assembly: Application to Hepatitis B Virus-Like Particles. 2022 , 23, 14699	0
56	Approaches and Perspective of Coarse-Grained Modeling and Simulation for Polymer-Nanoparticle Hybrid Systems. 2022 , 7, 47567-47586	0
55	NDP52 acts as a redox sensor in PINK1/Parkin-mediated mitophagy.	1
54	Predicting the Assembly of the Transmembrane Domains of Viral Channel Forming Proteins and Peptide Drug Screening Using a Docking Approach. 2022 , 12, 1844	0
53	Encapsulation of Gold-Based Anticancer Agents in Protease-Degradable Peptide Nanofilaments Enhances Their Potency.	0

- 52 Modeling of flexible membrane-bound biomolecular complexes for solution small-angle scattering. **2022**, ○
- 51 Evolution of β Peptide Self-Assembly: From Understanding to Prediction and Control. **2022**, 38, 15463-15475 ○
- 50 Comparative Study of Receptor-, Receptor State-, and Membrane-Dependent Cholesterol Binding Sites in A2A and A1 Adenosine Receptors Using Coarse-Grained Molecular Dynamics Simulations. ○
- 49 In Silico Analysis of Nanoplastics and β -amyloid Fibrils Interactions. **2023**, 28, 388 ○
- 48 Generating a conformational landscape of ubiquitin chains at atomistic resolution by back-mapping based sampling. 10, ○
- 47 Artificial extracellular matrix scaffolds of mobile molecules enhance maturation of human stem cell-derived neurons. **2023**, ○
- 46 Molecular Modeling Insights into the Structure and Behavior of Integrins: A review. **2023**, 12, 324 ○
- 45 CLIP-Seq Analysis Enables the Design of Ribosomal RNA Bait Oligonucleotides That Protect Against C9ORF72ALS/FTD-Associated Poly-GR Pathophysiology. ○
- 44 Facilitating CG Simulations with MAD: The MArtini Database Server. ○
- 43 Computer Simulation Techniques for Modelling Statics and Dynamics of Nanoscale Structures. **2014**, 230-299 ○
- 42 Particle-based mesoscale modeling and coarse-graining methods. **2023**, 75-111 ○
- 41 Development of a Data-driven Integrative Model of Bacterial Chromosome. ○
- 40 ProtRAP: Predicting Lipid Accessibility Together with Solvent Accessibility of Proteins in One Run. ○
- 39 A Top-down and Bottom-up Combined Strategy for Parameterization of Coarse-grained Force Fields for Phospholipids ○
- 38 A Diphenylalanine Based Pentapeptide with Fibrillating Self-Assembling Properties. **2023**, 15, 371 ○
- 37 pH-Dependent Conformational Switch Impacts Stability of the PsbS Dimer. **2023**, 14, 905-911 ○
- 36 A hybrid approach for coarse-graining helical peptoids: Solvation, secondary structure, and assembly. **2023**, 158, 114105 ○
- 35 Room for improvement in the initial martini 3 parameterization of peptide interactions. **2023**, 819, 140436 ○

- 34 Lipid domain boundary triggers membrane damage and protein folding of human islet amyloid polypeptide in the early pathogenesis of amyloid diseases. **2023**, 296, 106993 ○
- 33 The confluence of machine learning and multiscale simulations. **2023**, 80, 102569 ○
- 32 Computational insight into stability-enhanced systems of anthocyanin with protein/peptide. **2023**, 6, 100168 ○
- 31 Uncovering the mechanisms of cyclic peptide self-assembly in membranes with the chirality-aware MA(R/S)TINI forcefield. **2023**, 642, 84-99 ○
- 30 Enhanced antifouling properties of marine antimicrobial peptides by PEGylation. 11, ○
- 29 Protein Crowding and Cholesterol Increase Cell Membrane Viscosity in a Temperature Dependent Manner. ○
- 28 Elucidating activation and deactivation dynamics of VEGFR-2 transmembrane domain with coarse-grained molecular dynamics simulations. **2023**, 18, e0281781 ○
- 27 Structural basis for membrane attack complex inhibition by CD59. **2023**, 14, ○
- 26 Utilizing Machine Learning to Greatly Expand the Range and Accuracy of Bottom-Up Coarse-Grained Models through Virtual Particles. 1
- 25 Binding of SARS-CoV-2 non-structured protein 1 to 40S ribosome inhibits mRNA translation. ○
- 24 Immunoglobulin adsorption and film formation on mechanically wrinkled and crumpled surfaces at submonolayer coverage. **2023**, 5, 2085-2095 ○
- 23 Fluids and Electrolytes under Confinement in Single-Digit Nanopores. **2023**, 123, 2737-2831 ○
- 22 Lipid Bicelles in the Study of Biomembrane Characteristics. **2023**, 19, 1908-1921 ○
- 21 Direct determination of oligomeric organization of integral membrane proteins and lipids from intact customizable bilayer. ○
- 20 Mitigation of membrane morphology defects explain stability and orientational specificity of CLC dimers. ○
- 19 Machines on Genes through the Computational Microscope. **2023**, 19, 1945-1964 ○
- 18 Effective Molecular Dynamics from Neural Network-Based Structure Prediction Models. **2023**, 19, 1965-1975 ○
- 17 Folding and modulation of the helical conformation of Glycophorin A by point mutations. **2023**, 25, 10885-10893 ○

- 16 Solvent-controlled self-assembly of Fmoc protected aliphatic amino acids. ○
- 15 CHARMM-GUI Membrane Builder: Past, Current, and Future Developments and Applications. ○
- 14 Strategies to Prevent Water Soluble Drug Leakage from Nanovesicles in Blood Circulation: A Coarse-Grained Molecular Study. **2023**, 118715 ○
- 13 Coarse-Grained MD Simulations of Opioid Interactions with the μ Opioid Receptor and the Surrounding Lipid Membrane. **2023**, 3, 263-275 ○
- 12 Performance efficient macromolecular mechanics via sub-nanometer shape based coarse graining. **2023**, 14, ○
- 11 PMIpred: A physics-informed web server for quantitative Protein-Membrane Interaction prediction. ○
- 10 Optimizing the Martini 3 Force Field Reveals the Effects of the Intricate Balance between Protein-Water Interaction Strength and Salt Concentration on Biomolecular Condensate Formation. ○
- 9 An Efficient Method to Generate Dense Amorphous Structures for Molecular Simulation of Vinyl Polymers. **2023**, 408, ○
- 8 Protein Crowding and Cholesterol Increase Cell Membrane Viscosity in a Temperature Dependent Manner. ○
- 7 Machine Learning-Driven Multiscale Modeling: Bridging the Scales with a Next-Generation Simulation Infrastructure. ○
- 6 Development of a Data-Driven Integrative Model of a Bacterial Chromosome. ○
- 5 Theoretical Modeling of Self-Assembled Nanostructures of Amphiphiles in Solution. **2023**, 1161-1196 ○
- 4 Seipin concentrates distinct neutral lipids via interactions with their acyl chain carboxyl esters. **2022**, 221, ○
- 3 Visualizing the disordered nuclear transport machinery in situ. **2023**, 617, 162-169 ○
- 2 Anionic phospholipids stimulate the proton pumping activity of the plant plasma membrane P-type H^+ -ATPase. ○
- 1 N-Acetylation of Biodegradable Supramolecular Peptide Nanofilaments Selectively Enhances Their Proteolytic Stability for Targeted Delivery of Gold-Based Anticancer Agents. ○