

Optimization of the Additive CHARMM All-Atom Protein Force Field Sampling of the Backbone ϕ , ψ and Side-Chain χ_1

Journal of Chemical Theory and Computation

8, 3257-3273

DOI: 10.1021/ct300400x

Citation Report

#	ARTICLE	IF	CITATIONS
59	Automation of the CHARMM General Force Field (CGenFF) I: Bond Perception and Atom Typing. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 3144-3154.	2.5	1,409
60	Inclusion of Many-Body Effects in the Additive CHARMM Protein CMAP Potential Results in Enhanced Cooperativity of I [±] -Helix and I ² -Hairpin Formation. <i>Biophysical Journal</i> , 2012, 103, 1045-1051.	0.2	130
61	CHARMM36 all-atom additive protein force field: Validation based on comparison to NMR data. <i>Journal of Computational Chemistry</i> , 2013, 34, 2135-2145.	1.5	2,613
62	Efficient Determination of Protein-Protein Standard Binding Free Energies from First Principles. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3789-3798.	2.3	188
63	Polarizable Atomic Multipole-Based AMOEBA Force Field for Proteins. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4046-4063.	2.3	524
64	Systematic Improvement of a Classical Molecular Model of Water. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9956-9972.	1.2	279
65	Perspective: Coarse-grained models for biomolecular systems. <i>Journal of Chemical Physics</i> , 2013, 139, 090901.	1.2	675
66	Polarizable Force Field for Peptides and Proteins Based on the Classical Drude Oscillator. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5430-5449.	2.3	329
67	Dynamic Heterogeneous Dielectric Generalized Born (DHDGB): An Implicit Membrane Model with a Dynamically Varying Bilayer Thickness. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1709-1719.	2.3	43
68	PRIMO: A Transferable Coarse-Grained Force Field for Proteins. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3769-3788.	2.3	87
69	Predicting the Thermodynamics and Kinetics of Helix Formation in a Cyclic Peptide Model. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5148-5157.	2.3	28
70	Role of Water and Ions on the Dynamical Transition of RNA. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 3325-3329.	2.1	11
71	Molecular modeling of butyrylcholinesterase inhibition by cresyl saligenin phosphate. <i>Russian Chemical Bulletin</i> , 2013, 62, 2527-2537.	0.4	17
72	Effects of viscosity and osmotic stress on the reaction of human butyrylcholinesterase with cresyl saligenin phosphate, a toxicant related to aerotoxic syndrome: kinetic and molecular dynamics studies. <i>Biochemical Journal</i> , 2013, 454, 387-399.	1.7	53
73	Critical Assessment of Current Force Fields. Short Peptide Test Case. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 441-451.	2.3	29
74	A Simplified Confinement Method for Calculating Absolute Free Energies and Free Energy and Entropy Differences. <i>Journal of Physical Chemistry B</i> , 2013, 117, 750-762.	1.2	30
75	Protein Structure Refinement through Structure Selection and Averaging from Molecular Dynamics Ensembles. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1294-1303.	2.3	85
76	Molecular Basis of Cannabinoid CB1 Receptor Coupling to the G Protein Heterotrimer G _i 1 ² 3. <i>Journal of Biological Chemistry</i> , 2013, 288, 32449-32465.	1.6	24

#	ARTICLE	IF	CITATIONS
77	Two-Dimensional Infrared (2DIR) Spectroscopy of the Peptide Beta3s Folding. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1913-1917.	2.1	5
78	Molecular Details of the Activation of the $\frac{1}{4}$ Opioid Receptor. <i>Journal of Physical Chemistry B</i> , 2013, 117, 7907-7917.	1.2	28
79	Standard Binding Free Energies from Computer Simulations: What Is the Best Strategy?. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 794-802.	2.3	298
80	MODYLAS: A Highly Parallelized General-Purpose Molecular Dynamics Simulation Program for Large-Scale Systems with Long-Range Forces Calculated by Fast Multipole Method (FMM) and Highly Scalable Fine-Grained New Parallel Processing Algorithms. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3201-3209.	2.3	85
81	Replica-Averaged Metadynamics. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5610-5617.	2.3	64
82	Variational Optimization of an All-Atom Implicit Solvent Force Field To Match Explicit Solvent Simulation Data. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5641-5652.	2.3	46
83	Automated Optimization of Potential Parameters. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3311-3320.	2.3	32
84	Targeting Protein Tyrosine Phosphatase SHP2 for the Treatment of <i>PTPN11</i> -Associated Malignancies. <i>Molecular Cancer Therapeutics</i> , 2013, 12, 1738-1748.	1.9	41
85	Small Molecule Antivirulents Targeting the Iron-Regulated Heme Oxygenase (HemO) of <i>P. aeruginosa</i> . <i>Journal of Medicinal Chemistry</i> , 2013, 56, 2097-2109.	2.9	27
86	Insertion of the Ca ²⁺ -Independent Phospholipase A2 into a Phospholipid Bilayer via Coarse-Grained and Atomistic Molecular Dynamics Simulations. <i>PLoS Computational Biology</i> , 2013, 9, e1003156.	1.5	33
87	Turning Defense into Offense: Defensin Mimetics as Novel Antibiotics Targeting Lipid II. <i>PLoS Pathogens</i> , 2013, 9, e1003732.	2.1	50
88	(Ala) ₄ as a model system for the optimization of the ϕ and ψ amino acid side chain dihedral empirical force field parameters. <i>Journal of Computational Chemistry</i> , 2013, 34, 593-603.	1.5	5
89	Misplaced helix slows down ultrafast pressure-jump protein folding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 8087-8092.	3.3	51
90	Validating a Coarse-Grained Potential Energy Function through Protein Loop Modelling. <i>PLoS ONE</i> , 2013, 8, e65770.	1.1	14
91	Conformational Dynamics of a Ligand-Free Adenylate Kinase. <i>PLoS ONE</i> , 2013, 8, e68023.	1.1	27
92	Microsecond Molecular Dynamics Simulations of Mg ²⁺ - and K ⁺ - Bound E1 Intermediate States of the Calcium Pump. <i>PLoS ONE</i> , 2014, 9, e95979.	1.1	39
93	Ultrastable cellulosome-adhesion complex tightens under load. <i>Nature Communications</i> , 2014, 5, 5635.	5.8	92
94	Folding simulation of Trp-cage utilizing a new AMBER compatible force field with coupled main chain torsions. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450026.	1.8	6

#	ARTICLE	IF	CITATIONS
95	Conserved Allosteric Hot Spots in the Transmembrane Domains of Cystic Fibrosis Transmembrane Conductance Regulator (CFTR) Channels and Multidrug Resistance Protein (MRP) Pumps. <i>Journal of Biological Chemistry</i> , 2014, 289, 19942-19957.	1.6	20
96	Side-chain conformation at the selectivity filter shapes the permeation free-energy landscape of an ion channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, E3196-205.	3.3	16
97	Measurements and calculations of protein intramolecular vibrations in the THz range. , 2014, , .		3
98	Enhanced sampling simulations of DNA step parameters. <i>Journal of Computational Chemistry</i> , 2014, 35, 2297-2304.	1.5	17
99	Valence state parameters of all transition metal atoms in metalloproteinsâ€”development of ABEEMĭfĭ€ fluctuating charge force field. <i>Journal of Computational Chemistry</i> , 2014, 35, 1690-1706.	1.5	30
100	Recent Advances in Transferable Coarse-Grained Modeling of Proteins. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014, 96, 143-180.	1.0	46
101	Systematic Improvement of Potential-Derived Atomic Multipoles and Redundancy of the Electrostatic Parameter Space. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5493-5504.	2.3	30
102	Optical Signature of Formation of Protein Corona in the Firefly Luciferase-CdSe Quantum Dot Complex. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5224-5228.	2.3	16
103	Investigations of Ĩ±-helixĭ”ĭ²-sheet transition pathways in a miniprotein using the finite-temperature string method. <i>Journal of Chemical Physics</i> , 2014, 140, 175103.	1.2	21
104	Learning To Fold Proteins Using Energy Landscape Theory. <i>Israel Journal of Chemistry</i> , 2014, 54, 1311-1337.	1.0	57
105	Development and use of an atomistic CHARMM-based forcefield for peptoid simulation. <i>Journal of Computational Chemistry</i> , 2014, 35, 360-370.	1.5	67
106	An Electrostatic Interaction at the Tetrahelix Bundle Promotes Phosphorylation-dependent Cystic Fibrosis Transmembrane Conductance Regulator (CFTR) Channel Opening. <i>Journal of Biological Chemistry</i> , 2014, 289, 30364-30378.	1.6	33
107	Bayesian Energy Landscape Tilting: Towards Concordant Models of Molecular Ensembles. <i>Biophysical Journal</i> , 2014, 106, 1381-1390.	0.2	58
108	Insights into the binding of intrinsically disordered proteins from molecular dynamics simulation. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 182-198.	6.2	56
109	Protocol To Make Protein NMR Structures Amenable to Stable Long Time Scale Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1781-1787.	2.3	8
110	How Accurate Are Transition States from Simulations of Enzymatic Reactions?. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1863-1871.	2.3	21
111	Salt effects on hydrophobicĭ€core formation in folding of a helical miniprotein studied by molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 933-943.	1.5	3
112	Thermodynamics of Deca-alanine Folding in Water. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2836-2844.	2.3	44

#	ARTICLE	IF	CITATIONS
113	Interactions Outside the Proteinase-binding Loop Contribute Significantly to the Inhibition of Activated Coagulation Factor XII by Its Canonical Inhibitor from Corn. <i>Journal of Biological Chemistry</i> , 2014, 289, 14109-14120.	1.6	9
114	Simulations of remote mutants of dihydrofolate reductase reveal the nature of a network of residues coupled to hydride transfer. <i>Journal of Computational Chemistry</i> , 2014, 35, 1411-1417.	1.5	20
115	Molecular Modeling Evidence for His438 Flip in the Mechanism of Butyrylcholinesterase Hysteretic Behavior. <i>Journal of Molecular Neuroscience</i> , 2014, 52, 434-445.	1.1	14
116	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, 676-690.	2.3	566
117	Structural Plasticity in the Topology of the Membrane-Interacting Domain of HIV-1 gp41. <i>Biophysical Journal</i> , 2014, 106, 610-620.	0.2	22
118	The scaled-charge additive force field for amino acid based ionic liquids. <i>Chemical Physics Letters</i> , 2014, 616-617, 205-211.	1.2	41
119	Molecular Dynamics Study of Surfactant-Like Peptide Based Nanostructures. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12215-12222.	1.2	49
120	Balanced Protein-Water Interactions Improve Properties of Disordered Proteins and Non-Specific Protein Association. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5113-5124.	2.3	564
121	Assessing the hydration free energy of a homologous series of polyols with classical and quantum mechanical solvation models. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17863-17868.	1.3	2
122	How Accurately Do Current Force Fields Predict Experimental Peptide Conformations? An Adiabatic Free Energy Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6539-6552.	1.2	33
123	Spontaneous Self-Assembly of Engineered Armadillo Repeat Protein Fragments into a Folded Structure. <i>Structure</i> , 2014, 22, 985-995.	1.6	19
124	Three-dimensional protein structure prediction: Methods and computational strategies. <i>Computational Biology and Chemistry</i> , 2014, 53, 251-276.	1.1	160
125	Characterization of a novel butyrylcholinesterase point mutation (p.Ala34Val), <i>in silico</i> with mivacurium. <i>Biochemical Pharmacology</i> , 2014, 92, 476-483.	2.0	27
126	CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014, 96, 235-265.	1.0	214
127	Residue-Specific Force Field Based on the Protein Coil Library. RSFF1: Modification of OPLS-AA/L. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6983-6998.	1.2	93
128	Atomistic Description of Fullerene-Based Membranes. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12471-12477.	1.2	6
129	Induction of Peptide Bond Dipoles Drives Cooperative Helix Formation in the (AAQAA) ₃ Peptide. <i>Biophysical Journal</i> , 2014, 107, 991-997.	0.2	76
130	Conformational Changes and Free Energies in a Proline Isomerase. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4169-4174.	2.3	46

#	ARTICLE	IF	CITATIONS
131	ff14ipq: A Self-Consistent Force Field for Condensed-Phase Simulations of Proteins. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4515-4534.	2.3	87
132	Challenges in computational studies of enzyme structure, function and dynamics. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 54, 62-79.	1.3	50
133	CHARMM All-Atom Additive Force Field for Sphingomyelin: Elucidation of Hydrogen Bonding and of Positive Curvature. <i>Biophysical Journal</i> , 2014, 107, 134-145.	0.2	192
134	Terminal sialic acids on CD44 N-glycans can block hyaluronan binding by forming competing intramolecular contacts with arginine sidechains. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 3079-3089.	1.5	34
135	Density functional tight binding: values of semi-empirical methods in an ab initio era. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14368-14377.	1.3	125
136	Molecular Description of Surfactant-like Peptide Based Membranes. <i>Journal of Physical Chemistry C</i> , 2014, 118, 9598-9603.	1.5	29
137	Accelerate Sampling in Atomistic Energy Landscapes Using Topology-Based Coarse-Grained Models. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 918-923.	2.3	41
138	Optimizing Protein-Protein van der Waals Interactions for the AMBER ff9x/ff12 Force Field. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 273-281.	2.3	23
139	Computational Investigation of Cholesterol Binding Sites on Mitochondrial VDAC. <i>Journal of Physical Chemistry B</i> , 2014, 118, 9852-9860.	1.2	43
140	The VP4 Peptide of Hepatitis A Virus Ruptures Membranes through Formation of Discrete Pores. <i>Journal of Virology</i> , 2014, 88, 12409-12421.	1.5	38
141	Loss of conformational entropy in protein folding calculated using realistic ensembles and its implications for NMR-based calculations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 15396-15401.	3.3	101
142	Molecular dynamics study of enhanced Man5B enzymatic activity. <i>Biotechnology for Biofuels</i> , 2014, 7, 83.	6.2	36
143	Predicting the properties of a new class of host-guest complexes: C ₆₀ fullerene and CB[9] cucurbituril. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22823-22829.	1.3	20
144	Predicting the side-chain dihedral angle distributions of nonpolar, aromatic, and polar amino acids using hard sphere models. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 2574-2584.	1.5	21
145	Folding of Fourteen Small Proteins with a Residue-Specific Force Field and Replica-Exchange Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 2014, 136, 9536-9539.	6.6	66
146	Two Structural Scenarios for Protein Stabilization by PEG. <i>Journal of Physical Chemistry B</i> , 2014, 118, 8388-8395.	1.2	41
147	Mechanism of the pH-Controlled Self-Assembly of Nanofibers from Peptide Amphiphiles. <i>Journal of Physical Chemistry C</i> , 2014, 118, 16272-16278.	1.5	52
148	De novo inference of protein function from coarse-grained dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 2443-2454.	1.5	8

#	ARTICLE	IF	CITATIONS
149	Exploring Free-Energy Landscapes of Intrinsically Disordered Proteins at Atomic Resolution Using NMR Spectroscopy. <i>Chemical Reviews</i> , 2014, 114, 6632-6660.	23.0	252
150	Assessing the accuracy of physical models used in protein-folding simulations: quantitative evidence from long molecular dynamics simulations. <i>Current Opinion in Structural Biology</i> , 2014, 24, 98-105.	2.6	424
151	Conformational Preferences of DNA in Reduced Dielectric Environments. <i>Journal of Physical Chemistry B</i> , 2014, 118, 10874-10881.	1.2	25
152	A Tail of Two Peptide Amphiphiles: Effect of Conjugation with Hydrophobic Polymer on Folding of Peptide Sequences. <i>Biomacromolecules</i> , 2014, 15, 3313-3320.	2.6	4
153	Uncovering pH-Dependent Transient States of Proteins with Buried Ionizable Residues. <i>Journal of the American Chemical Society</i> , 2014, 136, 8496-8499.	6.6	38
154	Building Force Fields: An Automatic, Systematic, and Reproducible Approach. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1885-1891.	2.1	400
155	Multiscale Free Energy Simulations: An Efficient Method for Connecting Classical MD Simulations to QM or QM/MM Free Energies Using Non-Boltzmann Bennett Reweighting Schemes. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1406-1419.	2.3	111
156	Statistical Mechanics of the Denatured State of a Protein Using Replica-Averaged Metadynamics. <i>Journal of the American Chemical Society</i> , 2014, 136, 8982-8991.	6.6	69
157	Molecular basis for pseudokinase-dependent autoinhibition of JAK2 tyrosine kinase. <i>Nature Structural and Molecular Biology</i> , 2014, 21, 579-584.	3.6	132
158	Physics-based protein structure refinement through multiple molecular dynamics trajectories and structure averaging. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 196-207.	1.5	100
159	A structural mechanism for bacterial autotransporter glycosylation by a dodecameric heptosyltransferase family. <i>ELife</i> , 2014, 3, .	2.8	30
160	ABSINTH Implicit Solvation Model and Force Field Paradigm for Use in Simulations of Intrinsically Disordered Proteins. , 2014, , 208-231.		0
161	Crystal Structures of SecYEG in Lipidic Cubic Phase Elucidate a Precise Resting and a Peptide-Bound State. <i>Cell Reports</i> , 2015, 13, 1561-1568.	2.9	58
162	Peptide Recognition Capabilities of Cellulose in Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 24404-24416.	1.5	16
163	GENESIS: a hybrid-parallel and multi-scale molecular dynamics simulator with enhanced sampling algorithms for biomolecular and cellular simulations. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2015, 5, 310-323.	6.2	166
164	Force-Field Representation of Biomolecular Systems. , 2015, , 45-77.		3
166	Constraint methods that accelerate free-energy simulations of biomolecules. <i>Journal of Chemical Physics</i> , 2015, 143, 243143.	1.2	1
167	Energy landscape of LeuT from molecular simulations. <i>Journal of Chemical Physics</i> , 2015, 143, 243134.	1.2	34

#	ARTICLE	IF	CITATIONS
168	Structural Mechanism for Regulation of Bcl-2 protein Noxa by phosphorylation. Scientific Reports, 2015, 5, 14557.	1.6	11
169	Construction of a novel coarse grain model for simulations of HIV capsid assembly to capture the backbone structure and inter-domain motions in solution. Data in Brief, 2015, 5, 506-512.	0.5	9
170	Pressure-induced structural transition of mature HIV-1 protease from a combined NMR/MD simulation approach. Proteins: Structure, Function and Bioinformatics, 2015, 83, 2117-2123.	1.5	21
171	Self-Assembled Peptide-Polyfluorene Nanocomposites for Biodegradable Organic Electronics. Advanced Materials Interfaces, 2015, 2, 1500265.	1.9	35
172	Mechanism of lignin inhibition of enzymatic biomass deconstruction. Biotechnology for Biofuels, 2015, 8, 217.	6.2	195
173	Implementation of extended Langevin dynamics in GROMACS for polarizable simulations using the classical Drude oscillator model. Journal of Computational Chemistry, 2015, 36, 1473-1479.	1.5	79
174	Computational modeling of the N-terminus of the human dopamine transporter and its interaction with PIP ₂ -containing membranes. Proteins: Structure, Function and Bioinformatics, 2015, 83, 952-969.	1.5	47
175	Towards molecular modeling of the impact of heparin-derived oligosaccharides on hFN-1 binding. AIP Conference Proceedings, 2015, . .	0.3	1
176	New QM/MM implementation of the DFTB3 method in the gromacs package. Journal of Computational Chemistry, 2015, 36, 1978-1989.	1.5	45
177	Parametrization of macrolide antibiotics using the force field toolkit. Journal of Computational Chemistry, 2015, 36, 2052-2063.	1.5	15
178	Replica state exchange metadynamics for improving the convergence of free energy estimates. Journal of Computational Chemistry, 2015, 36, 1446-1455.	1.5	18
179	Enhanced stability of the model mini-protein in amino acid ionic liquids and their aqueous solutions. Journal of Computational Chemistry, 2015, 36, 2044-2051.	1.5	35
180	Structural integrity of the ribonuclease H domain in HIV-1 reverse transcriptase. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1526-1538.	1.5	6
181	Microsecond simulations of mdm2 and its complex with p53 yield insight into force field accuracy and conformational dynamics. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1665-1676.	1.5	24
182	Integrating atomistic molecular dynamics simulations, experiments, and network analysis to study protein dynamics: strength in unity. Frontiers in Molecular Biosciences, 2015, 2, 28.	1.6	64
183	Comparing Molecular Dynamics Force Fields in the Essential Subspace. PLoS ONE, 2015, 10, e0121114.	1.1	80
184	New Infestin-4 Mutants with Increased Selectivity against Factor XIIa. PLoS ONE, 2015, 10, e0144940.	1.1	17
185	Motion Tree Delineates Hierarchical Structure of Protein Dynamics Observed in Molecular Dynamics Simulation. PLoS ONE, 2015, 10, e0131583.	1.1	19

#	ARTICLE	IF	CITATIONS
186	Uncovering Molecular Bases Underlying Bone Morphogenetic Protein Receptor Inhibitor Selectivity. PLoS ONE, 2015, 10, e0132221.	1.1	11
187	Conformational Changes in Two Inter-Helical Loops of Mhp1 Membrane Transporter. PLoS ONE, 2015, 10, e0133388.	1.1	11
188	Monoamine transporters: insights from molecular dynamics simulations. Frontiers in Pharmacology, 2015, 6, 235.	1.6	60
189	Structure–activity exploration of a small-molecule Lipid II inhibitor. Drug Design, Development and Therapy, 2015, 9, 2383.	2.0	7
190	Microseconds Simulations Reveal a New Sodium-binding Site and the Mechanism of Sodium-coupled Substrate Uptake by LeuT. Journal of Biological Chemistry, 2015, 290, 544-555.	1.6	48
191	Microsecond Molecular Simulations Reveal a Transient Proton Pathway in the Calcium Pump. Journal of the American Chemical Society, 2015, 137, 7055-7058.	6.6	18
192	A Combined NMR and Computational Approach to Investigate Peptide Binding to a Designed Armadillo Repeat Protein. Journal of Molecular Biology, 2015, 427, 1916-1933.	2.0	6
193	Conformational Dynamics of Two Natively Unfolded Fragment Peptides: Comparison of the AMBER and CHARMM Force Fields. Journal of Physical Chemistry B, 2015, 119, 7902-7910.	1.2	16
194	Conformational Changes of the Clamp of the Protein Translocation ATPase SecA. Journal of Molecular Biology, 2015, 427, 2348-2359.	2.0	26
195	The force field for imidazolium-based ionic liquids: Novel anions with polar residues. Chemical Physics Letters, 2015, 633, 132-138.	1.2	13
196	Complete atomistic model of a bacterial cytoplasm for integrating physics, biochemistry, and systems biology. Journal of Molecular Graphics and Modelling, 2015, 58, 1-9.	1.3	71
197	The Origin of Consistent Protein Structure Refinement from Structural Averaging. Structure, 2015, 23, 1123-1128.	1.6	16
198	Sarcolipin and phospholamban inhibit the calcium pump by populating a similar metal ion-free intermediate state. Biochemical and Biophysical Research Communications, 2015, 463, 37-41.	1.0	31
199	High-resolution structures of the M2 channel from influenza A virus reveal dynamic pathways for proton stabilization and transduction. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 14260-14265.	3.3	92
200	Induced Dipole–Dipole Interactions Influence the Unfolding Pathways of Wild-Type and Mutant Amyloid β -Peptides. Journal of Physical Chemistry B, 2015, 119, 15574-15582.	1.2	30
201	The Crystal Structure of an Integral Membrane Fatty Acid β -Hydroxylase. Journal of Biological Chemistry, 2015, 290, 29820-29833.	1.6	52
202	Mutational and Computational Evidence That a Nickel-Transfer Tunnel in UreD Is Used for Activation of <i>Klebsiella aerogenes</i> Urease. Biochemistry, 2015, 54, 6392-6401.	1.2	41
203	Structural insights into the DNA-binding specificity of E2F family transcription factors. Nature Communications, 2015, 6, 10050.	5.8	43

#	ARTICLE	IF	CITATIONS
204	Effect of O-Linked Glycosylation on the Equilibrium Structural Ensemble of Intrinsically Disordered Polypeptides. <i>Journal of Physical Chemistry B</i> , 2015, 119, 15583-15592.	1.2	19
205	Structural Properties of Protein-Detergent Complexes from SAXS and MD Simulations. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 5116-5121.	2.1	25
206	Atomistic Characterization of the First Step of Calcium Pump Activation Associated with Proton Countertransport. <i>Biochemistry</i> , 2015, 54, 5235-5241.	1.2	9
207	Interaction of cisplatin and two potential antitumoral platinum(II) complexes with a model lipid membrane: a combined NMR and MD study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 1458-1468.	1.3	16
208	Prediction of the structures of helical membrane proteins based on a minimum unfavorable contacts approach. <i>Journal of Computational Chemistry</i> , 2015, 36, 539-552.	1.5	3
209	Membrane association of the PTEN tumor suppressor: Neutron scattering and MD simulations reveal the structure of protein-membrane complexes. <i>Methods</i> , 2015, 77-78, 136-146.	1.9	28
210	Current Status of Protein Force Fields for Molecular Dynamics Simulations. <i>Methods in Molecular Biology</i> , 2015, 1215, 47-71.	0.4	139
211	REIN: Replica-Exchange Interface for simulating protein dynamics and function. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 325-332.	1.0	3
212	Evolutionary Conserved Tyr169 Stabilizes the $\beta 2-\beta 2$ Loop of the Prion Protein. <i>Journal of the American Chemical Society</i> , 2015, 137, 2948-2957.	6.6	36
213	Spatial Analysis and Quantification of the Thermodynamic Driving Forces in Protein-Ligand Binding: Binding Site Variability. <i>Journal of the American Chemical Society</i> , 2015, 137, 2608-2621.	6.6	21
214	Interactions of Amino Acid Side-Chain Analogs within Membrane Environments. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2877-2885.	1.2	16
215	Simulating the Distance Distribution between Spin-Labels Attached to Proteins. <i>Journal of Physical Chemistry B</i> , 2015, 119, 3901-3911.	1.2	46
216	Molecular Dynamics Simulations of Heart-type Fatty Acid Binding Protein in Apo and Holo Forms, and Hydration Structure Analyses in the Binding Cavity. <i>Journal of Physical Chemistry B</i> , 2015, 119, 114-127.	1.2	26
217	Residue-Specific Force Field Based on Protein Coil Library. RSFF2: Modification of AMBER ff99SB. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1035-1047.	1.2	92
218	Conformational Sampling of Oligosaccharides Using Hamiltonian Replica Exchange with Two-Dimensional Dihedral Biasing Potentials and the Weighted Histogram Analysis Method (WHAM). <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 788-799.	2.3	38
219	Five checkpoints maintaining the fidelity of transcription by RNA polymerases in structural and energetic details. <i>Nucleic Acids Research</i> , 2015, 43, 1133-1146.	6.5	24
220	Identification of a novel carbohydrate esterase from <i>Bjerkandera adusta</i> : Structural and function predictions through bioinformatics analysis and molecular modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 533-546.	1.5	6
221	A PDI-catalyzed thiol-disulfide switch regulates the production of hydrogen peroxide by human Ero1. <i>Free Radical Biology and Medicine</i> , 2015, 83, 361-372.	1.3	59

#	ARTICLE	IF	CITATIONS
222	In vitro human serum albumin glycation monitored by Terahertz spectroscopy. <i>Optical and Quantum Electronics</i> , 2015, 47, 961-973.	1.5	10
223	Claws, Disorder, and Conformational Dynamics of the C Terminal Region of Human Desmoplakin. <i>Biophysical Journal</i> , 2015, 108, 389a-390a.	0.2	0
224	Structural basis for chemokine recognition and activation of a viral G protein-coupled receptor. <i>Science</i> , 2015, 347, 1113-1117.	6.0	261
225	Role of the Fourth Transmembrane $\hat{\alpha}$ Helix in the Allosteric Modulation of Pentameric Ligand-Gated Ion Channels. <i>Structure</i> , 2015, 23, 1655-1664.	1.6	29
226	Nascent $\hat{\alpha}$ 2-Hairpin Formation of a Natively Unfolded Peptide Reveals the Role of Hydrophobic Contacts. <i>Biophysical Journal</i> , 2015, 109, 630-638.	0.2	6
227	Probing Site-Specific Structural Information of Peptides at Model Membrane Interface In Situ. <i>Journal of the American Chemical Society</i> , 2015, 137, 10190-10198.	6.6	51
228	Structural insights into $\hat{\mu}$ -opioid receptor activation. <i>Nature</i> , 2015, 524, 315-321.	13.7	743
229	Geometric rules of channel gating inferred from computational models of the P2X receptor transmembrane domain. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 61, 107-114.	1.3	2
230	Explaining the mobility of retinal in activated rhodopsin and opsin. <i>Photochemical and Photobiological Sciences</i> , 2015, 14, 1952-1964.	1.6	3
231	Are the Crystal Structures of Enantiopure and Racemic Mandelic Acids Determined by Kinetics or Thermodynamics?. <i>Journal of the American Chemical Society</i> , 2015, 137, 11095-11104.	6.6	57
232	Developing the IVIG biomimetic, Hexa-Fc, for drug and vaccine applications. <i>Scientific Reports</i> , 2015, 5, 9526.	1.6	33
233	Enhanced Sampling of an Atomic Model with Hybrid Nonequilibrium Molecular Dynamics Monte Carlo Simulations Guided by a Coarse-Grained Model. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3572-3583.	2.3	18
234	ff14SB: Improving the Accuracy of Protein Side Chain and Backbone Parameters from ff99SB. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3696-3713.	2.3	7,322
235	DNA Elasticity from Short DNA to Nucleosomal DNA. <i>Journal of Physical Chemistry B</i> , 2015, 119, 11146-11156.	1.2	48
236	Atomic Modeling of an Immature Retroviral Lattice Using Molecular Dynamics and Mutagenesis. <i>Structure</i> , 2015, 23, 1414-1425.	1.6	35
237	Insights into the Lactonase Mechanism of Serum Paraoxonase 1 (PON1): Experimental and Quantum Mechanics/Molecular Mechanics (QM/MM) Studies. <i>Journal of Physical Chemistry B</i> , 2015, 119, 9571-9585.	1.2	7
238	Regulating Ion Transport in Peptide Nanotubes by Tailoring the Nanotube Lumen Chemistry. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1514-1520.	2.1	14
239	How osmolytes influence hydrophobic polymer conformations: A unified view from experiment and theory. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 9270-9275.	3.3	98

#	ARTICLE	IF	CITATIONS
240	Biomembranes in atomistic and coarse-grained simulations. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 323103.	0.7	61
241	Chromatin Unfolding by Epigenetic Modifications Explained by Dramatic Impairment of Internucleosome Interactions: A Multiscale Computational Study. <i>Journal of the American Chemical Society</i> , 2015, 137, 10205-10215.	6.6	135
242	Correct folding of an α -helix and a β -hairpin using a polarized 2D torsional potential. <i>Scientific Reports</i> , 2015, 5, 10359.	1.6	15
243	Force field-dependent solution properties of glycine oligomers. <i>Journal of Computational Chemistry</i> , 2015, 36, 1275-1285.	1.5	26
244	Enhanced Conformational Sampling Using Replica Exchange with Concurrent Solute Scaling and Hamiltonian Biasing Realized in One Dimension. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2855-2867.	2.3	35
245	Determining protein structures by combining semireliable data with atomistic physical models by Bayesian inference. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 6985-6990.	3.3	132
246	Conserved water molecules in bacterial serine hydroxymethyltransferases. <i>Protein Engineering, Design and Selection</i> , 2015, 28, 415-426.	1.0	4
247	Mapping Functional Group Free Energy Patterns at Protein Occluded Sites: Nuclear Receptors and G-Protein Coupled Receptors. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 700-708.	2.5	48
248	Spontaneous Adsorption of Coiled-Coil Model Peptides K and E to a Mixed Lipid Bilayer. <i>Journal of Physical Chemistry B</i> , 2015, 119, 4396-4408.	1.2	29
249	Atomic-Level Mechanisms for Phospholamban Regulation of the Calcium Pump. <i>Biophysical Journal</i> , 2015, 108, 1697-1708.	0.2	35
250	Structural and biophysical characterization of an epitope-specific engineered Fab fragment and complexation with membrane proteins: implications for co-crystallization. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 896-906.	2.5	13
251	The influence of cholesterol on membrane protein structure, function, and dynamics studied by molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2015, 1848, 1783-1795.	1.4	144
252	Properties of an Inward-Facing State of LeuT: Conformational Stability and Substrate Release. <i>Biophysical Journal</i> , 2015, 108, 1390-1399.	0.2	26
253	Redox Potential Tuning through Differential Quinone Binding in the Photosynthetic Reaction Center of <i>Rhodobacter sphaeroides</i> . <i>Biochemistry</i> , 2015, 54, 2104-2116.	1.2	11
254	Efficient parametrization of complex molecule surface force fields. <i>Journal of Computational Chemistry</i> , 2015, 36, 1187-1195.	1.5	9
255	Structural basis for a novel mechanism of DNA bridging and alignment in eukaryotic DSB DNA repair. <i>EMBO Journal</i> , 2015, 34, 1126-1142.	3.5	21
256	The Structure of a Melittin-Stabilized Pore. <i>Biophysical Journal</i> , 2015, 108, 2424-2426.	0.2	64
257	Conformational Changes Underlying Desensitization of the Pentameric Ligand-Gated Ion Channel ELIC. <i>Structure</i> , 2015, 23, 995-1004.	1.6	38

#	ARTICLE	IF	CITATIONS
258	Acyl-2-aminobenzimidazoles: A novel class of neuroprotective agents targeting mGluR5. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 2211-2220.	1.4	21
259	Effects of N-glycosylation on protein conformation and dynamics: Protein Data Bank analysis and molecular dynamics simulation study. <i>Scientific Reports</i> , 2015, 5, 8926.	1.6	187
260	Ion Hydration Dynamics in Conjunction with a Hydrophobic Gating Mechanism Regulates Ion Permeation in p7 Viroprotein from Hepatitis C Virus. <i>Journal of Physical Chemistry B</i> , 2015, 119, 6204-6210.	1.2	9
261	Pushing the Limits of a Molecular Mechanics Force Field To Probe Weak CH π Interactions in Proteins. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1854-1863.	2.3	5
262	Systematic evaluation of bundled SPC water for biomolecular simulations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 8393-8406.	1.3	26
263	High-resolution structural characterization of Noxa, an intrinsically disordered protein, by microsecond molecular dynamics simulations. <i>Molecular BioSystems</i> , 2015, 11, 1850-1856.	2.9	7
264	Free Energy Surface of the Michaelis Complex of Lactate Dehydrogenase: A Network Analysis of Microsecond Simulations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 5430-5436.	1.2	11
265	Structural insights into the efficient CO ₂ -reducing activity of an NAD-dependent formate dehydrogenase from <i>Thiobacillus</i> sp. KNK65MA. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 313-323.	2.5	23
266	Molecular modeling of the human P2Y ₁₄ receptor: A template for structure-based design of selective agonist ligands. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 4056-4064.	1.4	24
267	Quantum Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4992-5001.	2.3	42
268	Theoretical demonstration of the potentiality of boron nitride nanotubes to encapsulate anticancer molecule. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30057-30064.	1.3	25
269	Dynamic properties of force fields. <i>Journal of Chemical Physics</i> , 2015, 142, 084101.	1.2	70
270	Resting state of the human proton channel dimer in a lipid bilayer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E5926-35.	3.3	68
271	The molecular mechanism of Zinc acquisition by the neisserial outer-membrane transporter ZnuD. <i>Nature Communications</i> , 2015, 6, 7996.	5.8	58
272	Structural Ensembles of Intrinsically Disordered Proteins Depend Strongly on Force Field: A Comparison to Experiment. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5513-5524.	2.3	368
273	Synaptobrevin Transmembrane Domain Dimerization Studied by Multiscale Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2015, 109, 760-771.	0.2	22
274	Toward a Whole-Cell Model of Ribosome Biogenesis: Kinetic Modeling of SSU Assembly. <i>Biophysical Journal</i> , 2015, 109, 1117-1135.	0.2	25
275	An Analysis of Biomolecular Force Fields for Simulations of Polyglutamine in Solution. <i>Biophysical Journal</i> , 2015, 109, 1009-1018.	0.2	40

#	ARTICLE	IF	CITATIONS
276	Dynamics of the BH3-Only Protein Binding Interface of Bcl-xL. <i>Biophysical Journal</i> , 2015, 109, 1049-1057.	0.2	11
277	Variational cross-validation of slow dynamical modes in molecular kinetics. <i>Journal of Chemical Physics</i> , 2015, 142, 124105.	1.2	173
278	Membrane Interaction of the Factor VIIIa Discoidin Domains in Atomistic Detail. <i>Biochemistry</i> , 2015, 54, 6123-6131.	1.2	20
279	Examining the Assumptions Underlying Continuum-Solvent Models. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4593-4600.	2.3	18
280	Polypeptide A9K at nanoscale carbon: a simulation study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 26386-26393.	1.3	4
281	A generic implementation of replica exchange with solute tempering (REST2) algorithm in NAMD for complex biophysical simulations. <i>Computer Physics Communications</i> , 2015, 197, 304-311.	3.0	54
282	Atomistic Glimpse of the Orderly Chaos of One Protein. <i>Biophysical Journal</i> , 2015, 109, 1511-1512.	0.2	0
283	Toward Automated Benchmarking of Atomistic Force Fields: Neat Liquid Densities and Static Dielectric Constants from the ThermoML Data Archive. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12912-12920.	1.2	30
284	pmx: Automated protein structure and topology generation for alchemical perturbations. <i>Journal of Computational Chemistry</i> , 2015, 36, 348-354.	1.5	199
285	MODYLAS: A highly parallelized general-purpose molecular dynamics simulation program. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 342-348.	1.0	4
286	Understanding the Reaction Mechanism and Intermediate Stabilization in Mammalian Serine Racemase Using Multiscale Quantum-Classical Simulations. <i>Biochemistry</i> , 2015, 54, 516-527.	1.2	12
287	Toward Molecular Mechanism of Xenon Anesthesia: A Link to Studies of Xenon Complexes with Small Aromatic Molecules. <i>Journal of Physical Chemistry A</i> , 2015, 119, 2517-2521.	1.1	11
288	Free Energy Simulations of Active-Site Mutants of Dihydrofolate Reductase. <i>Journal of Physical Chemistry B</i> , 2015, 119, 906-916.	1.2	20
289	Tailoring the water structure and transport in nanotubes with tunable interiors. <i>Nanoscale</i> , 2015, 7, 121-132.	2.8	46
290	CHARMM additive and polarizable force fields for biophysics and computer-aided drug design. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 861-871.	1.1	223
291	Effect of external pulling forces on the length distribution of peptides. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 903-910.	1.1	4
292	Effects of Cd ²⁺ on the epithelial Na ⁺ channel (ENaC) investigated by experimental and modeling studies. <i>General Physiology and Biophysics</i> , 2016, 35, 259-271.	0.4	1
293	Photo-switchable tweezers illuminate pore-opening motions of an ATP-gated P2X ion channel. <i>ELife</i> , 2016, 5, e11050.	2.8	31

#	ARTICLE	IF	CITATIONS
294	The Mutational Landscape of the Oncogenic MZF1 SCAN Domain in Cancer. <i>Frontiers in Molecular Biosciences</i> , 2016, 3, 78.	1.6	34
295	Jump into a New Fold—A Homology Based Model for the ABCG2/BCRP Multidrug Transporter. <i>PLoS ONE</i> , 2016, 11, e0164426.	1.1	45
296	Computational Tools for the Study of Biomolecules. <i>Computer Aided Chemical Engineering</i> , 2016, , 583-648.	0.3	7
297	Common Anesthetic-binding Site for Inhibition of Pentameric Ligand-gated Ion Channels. <i>Anesthesiology</i> , 2016, 124, 664-673.	1.3	14
298	Iminoguanidines as Allosteric Inhibitors of the Iron-Regulated Heme Oxygenase (HemO) of <i>Pseudomonas aeruginosa</i> . <i>Journal of Medicinal Chemistry</i> , 2016, 59, 6929-6942.	2.9	33
299	Pushing the Envelope: Dengue Viral Membrane Coaxed into Shape by Molecular Simulations. <i>Structure</i> , 2016, 24, 1410-1420.	1.6	41
300	DIRECT: An automated method to identify and quantify conformational variations—application to β_2 -adrenergic GPCR. <i>Journal of Computational Chemistry</i> , 2016, 37, 416-425.	1.5	13
301	Kainate receptor pore-forming and auxiliary subunits regulate channel block by a novel mechanism. <i>Journal of Physiology</i> , 2016, 594, 1821-1840.	1.3	24
302	Free energies of solvation in the context of protein folding: Implications for implicit and explicit solvent models. <i>Journal of Computational Chemistry</i> , 2016, 37, 629-640.	1.5	24
303	Protein structure refinement via molecular dynamics simulations: What works and what does not?. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 282-292.	1.5	60
304	Structural Correlation of the Neck Coil with the Coiled-coil (CC1)-Forkhead-associated (FHA) Tandem for Active Kinesin-3 KIF13A. <i>Journal of Biological Chemistry</i> , 2016, 291, 3581-3594.	1.6	9
305	Local Protein Structure Refinement via Molecular Dynamics Simulations with locPREFMD. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1304-1312.	2.5	65
306	Improved model of hydrated calcium ion for molecular dynamics simulations using classical biomolecular force fields. <i>Biopolymers</i> , 2016, 105, 752-763.	1.2	40
307	Quantifying electron transfer reactions in biological systems: what interactions play the major role?. <i>Scientific Reports</i> , 2016, 5, 18446.	1.6	67
308	Reciprocal voltage sensor-to-pore coupling leads to potassium channel C-type inactivation. <i>Scientific Reports</i> , 2016, 6, 27562.	1.6	18
309	Uncovering the Binding and Specificity of β_2 -Wrapins for Amyloid- β and β -Synuclein. <i>Journal of Physical Chemistry B</i> , 2016, 120, 12781-12794.	1.2	22
310	Molecular polymorphism of human enzymes as the basis of individual sensitivity to drugs. Supercomputer-assisted modeling as a tool for analysis of structural changes and enzymatic activity of proteins. <i>Russian Chemical Bulletin</i> , 2016, 65, 1592-1607.	0.4	8
311	Molecular dynamics simulation elucidates the preferential binding affinity of sodium and tetramethylammonium ions for tetrameric Nafion unit under aqueous conditions. <i>RSC Advances</i> , 2016, 6, 97961-97968.	1.7	6

#	ARTICLE	IF	CITATIONS
312	The allosteric switching mechanism in bacteriophage MS2. <i>Journal of Chemical Physics</i> , 2016, 145, 035101.	1.2	12
313	Characterizing the Conformational Landscape of Flavivirus Fusion Peptides via Simulation and Experiment. <i>Scientific Reports</i> , 2016, 6, 19160.	1.6	17
314	Mechanism of pH-dependent activation of the sodium-proton antiporter NhaA. <i>Nature Communications</i> , 2016, 7, 12940.	5.8	90
315	Structure-Based Scaffold Repurposing for G Protein-Coupled Receptors: Transformation of Adenosine Derivatives into 5HT _{2B} /5HT _{2C} Serotonin Receptor Antagonists. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 11006-11026.	2.9	18
316	Isolated pores dissected from human two-pore channel 2 are functional. <i>Scientific Reports</i> , 2016, 6, 38426.	1.6	9
317	Membrane Anchoring and Ion-Entry Dynamics in P-type ATPase Copper Transport. <i>Biophysical Journal</i> , 2016, 111, 2417-2429.	0.2	16
318	Cyclophilin A stabilizes the HIV-1 capsid through a novel non-canonical binding site. <i>Nature Communications</i> , 2016, 7, 10714.	5.8	126
319	Communication: Consistent interpretation of molecular simulation kinetics using Markov state models biased with external information. <i>Journal of Chemical Physics</i> , 2016, 144, 051102.	1.2	31
320	Molecular dynamics for irradiation driven chemistry: application to the FEBID process*. <i>European Physical Journal D</i> , 2016, 70, 1.	0.6	30
321	A first principle particle mesh method for solution SAXS of large bio-molecular systems. <i>Journal of Chemical Physics</i> , 2016, 145, 045101.	1.2	7
322	Tyrosine Templating in the Self-Assembly and Crystallization of Silk Fibroin. <i>Biomacromolecules</i> , 2016, 17, 3570-3579.	2.6	54
323	Novel Analogues of (<i>R</i>)-5-(Methylamino)-5,6-dihydro-4<i>H</i>-imidazo[4,5,1- <i>ij</i>]quinolin-2(1<i>H</i>)-one (Sumanriole) Provide Clues to Dopamine D₂/D₃ Receptor Agonist Selectivity. <i>Journal of Medicinal Chemistry</i>, 2016, 59, 2973-2988.</i>	2.9	33
324	Single-Molecule Chemo-Mechanical Spectroscopy Provides Structural Identity of Folding Intermediates. <i>Biophysical Journal</i> , 2016, 110, 1280-1290.	0.2	19
325	Molecular simulations of micellar aggregation of polysorbate 20 ester fractions and their interaction with N-phenyl-1-naphthylamine dye. <i>Biophysical Chemistry</i> , 2016, 213, 17-24.	1.5	19
326	Molecular dynamics simulation of triclinic lysozyme in a crystal lattice. <i>Protein Science</i> , 2016, 25, 87-102.	3.1	52
327	Recognition of Poly-Ubiquitins by the Proteasome through Protein Refolding Guided by Electrostatic and Hydrophobic Interactions. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8137-8146.	1.2	11
328	Exploring the Formation and the Structure of Synaptobrevin Oligomers in a Model Membrane. <i>Biophysical Journal</i> , 2016, 110, 2004-2015.	0.2	13
329	Trajectories of microsecond molecular dynamics simulations of nucleosomes and nucleosome core particles. <i>Data in Brief</i> , 2016, 7, 1678-1681.	0.5	3

#	ARTICLE	IF	CITATIONS
330	Validation of polarizable force field parameters for nucleic acids by inter-molecular interactions. <i>Frontiers of Chemical Science and Engineering</i> , 2016, 10, 203-212.	2.3	5
331	Fast calculation of molecular total energy with ABEEM π /MM method " For some series of organic molecules and peptides. <i>Chemical Physics</i> , 2016, 472, 24-35.	0.9	2
332	TopoGromacs: Automated Topology Conversion from CHARMM to GROMACS within VMD. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1112-1116.	2.5	63
333	Molecular Dynamics Simulations Reveal the Conformational Flexibility of Lipid II and Its Loose Association with the Defensin Plectasin in the <i>Staphylococcus aureus</i> Membrane. <i>Biochemistry</i> , 2016, 55, 3303-3314.	1.2	18
334	Contribution of Electrostatics to the Kinetics of Electron Transfer from NADH-Cytochrome b ₅ Reductase to Fe(III)-Cytochrome b ₅ . <i>Journal of Physical Chemistry B</i> , 2016, 120, 8193-8207.	1.2	5
335	The dynamics of the $\hat{\Gamma}^2$ -propeller domain in Kelch protein KLHL40 changes upon nemaline myopathy-associated mutation. <i>RSC Advances</i> , 2016, 6, 34043-34054.	1.7	6
336	Reconstructing the TIR Side of the Myddosome: a Paradigm for TIR-TIR Interactions. <i>Structure</i> , 2016, 24, 437-447.	1.6	63
337	How Does Hyperphosphorylation Promote Tau Aggregation and Modulate Filament Structure and Stability?. <i>ACS Chemical Neuroscience</i> , 2016, 7, 565-575.	1.7	27
338	CHARMM TIP3P Water Model Suppresses Peptide Folding by Solvating the Unfolded State. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3692-3698.	1.2	136
339	Protein Folding and Structure Prediction from the Ground Up: The Atomistic Associative Memory, Water Mediated, Structure and Energy Model. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8557-8565.	1.2	28
340	A Simple and Accurate Method To Calculate Free Energy Profiles and Reaction Rates from Restrained Molecular Simulations of Diffusive Processes. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8457-8472.	1.2	18
341	Accurate Structure Prediction and Conformational Analysis of Cyclic Peptides with Residue-Specific Force Fields. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1805-1810.	2.1	50
342	Transitions of Double-Stranded DNA Between the A- and B-Forms. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8449-8456.	1.2	38
343	Modeling the Complete Catalytic Cycle of Aspartoacylase. <i>Journal of Physical Chemistry B</i> , 2016, 120, 4221-4231.	1.2	25
344	Cooperation of Hydrophobic Gating, Knock-on Effect, and Ion Binding Determines Ion Selectivity in the p7 Channel. <i>Journal of Physical Chemistry B</i> , 2016, 120, 4351-4356.	1.2	5
345	Slow-binding inhibition of acetylcholinesterase by an alkylammonium derivative of 6-methyluracil: mechanism and possible advantages for myasthenia gravis treatment. <i>Biochemical Journal</i> , 2016, 473, 1225-1236.	1.7	39
346	X-ray Crystallographic Structure of Thermophilic Rhodopsin. <i>Journal of Biological Chemistry</i> , 2016, 291, 12223-12232.	1.6	38
347	Molecular mechanisms of endocrine and metabolic disruption: An in silico study on antitrypanosomal natural products and some derivatives. <i>Toxicology Letters</i> , 2016, 252, 29-41.	0.4	4

#	ARTICLE	IF	CITATIONS
348	Fusion peptide of HIV-1 as a site of vulnerability to neutralizing antibody. <i>Science</i> , 2016, 352, 828-833.	6.0	310
349	Molecular Dynamics Simulations to Study Structure-Function Relationship in Psychrophilic Enzymes. <i>Grand Challenges in Biology and Biotechnology</i> , 2016, , 675-698.	2.4	1
350	Meandering Down the Energy Landscape of Protein Folding: Are We There Yet?. <i>Biophysical Journal</i> , 2016, 110, 1924-1932.	0.2	16
352	Optimization of Protein Backbone Dihedral Angles by Means of Hamiltonian Reweighting. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1823-1834.	2.5	7
353	Structure and Dynamics of Extracellular Loops in Human Aquaporin-1 from Solid-State NMR and Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9887-9902.	1.2	24
354	Pharmacophore-based virtual screening, biological evaluation and binding mode analysis of a novel protease-activated receptor 2 antagonist. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 625-637.	1.3	3
355	Does Replica Exchange with Solute Tempering Efficiently Sample Δ^2 Peptide Conformational Ensembles?. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5201-5214.	2.3	47
356	Death Receptor 5 Networks Require Membrane Cholesterol for Proper Structure and Function. <i>Journal of Molecular Biology</i> , 2016, 428, 4843-4855.	2.0	15
357	Structure prediction and functional analysis of a non-permuted lectin from <i>Dioclea grandiflora</i> . <i>Biochimie</i> , 2016, 131, 54-67.	1.3	3
358	Domain Organization in the 54-kDa Subunit of the Chloroplast Signal Recognition Particle. <i>Biophysical Journal</i> , 2016, 111, 1151-1162.	0.2	7
359	FF12MC: A revised AMBER forcefield and new protein simulation protocol. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 1490-1516.	1.5	37
360	Conformational and electrostatic analysis of SN1 donor analogue glycomimetic inhibitors of ST3Gal-I mammalian sialyltransferase. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 4998-5005.	1.4	2
361	Role of the Native Outer-Membrane Environment on the Transporter BtuB. <i>Biophysical Journal</i> , 2016, 111, 1409-1417.	0.2	48
362	Intrinsic Base-Pair Rearrangement in the Hairpin Ribozyme Directs RNA Conformational Sampling and Tertiary Interface Formation. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10885-10898.	1.2	3
363	Molecular basis of the osmolyte effect on protein stability: a lesson from the mechanical unfolding of lysozyme. <i>Biochemical Journal</i> , 2016, 473, 3705-3724.	1.7	19
364	Estimating glycosaminoglycan-protein interaction affinity: water dominates the specific antithrombin-heparin interaction. <i>Glycobiology</i> , 2016, 26, 1041-1047.	1.3	19
365	Assessing the physiological relevance of alternate architectures of the p7 protein of hepatitis C virus in different environments. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 4920-4927.	1.4	9
366	Encapsulation capacity and natural payload delivery of an anticancer drug from boron nitride nanotube. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24994-25001.	1.3	49

#	ARTICLE	IF	CITATIONS
367	C-terminal tail insertion of Bcl-xL in membrane occurs via partial unfolding and refolding cycle associating microsolvation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24095-24105.	1.3	4
368	Distal Hydrogen-bonding Interactions in Ligand Sensing and Signaling by <i>Mycobacterium tuberculosis</i> DosS. <i>Journal of Biological Chemistry</i> , 2016, 291, 16100-16111.	1.6	17
369	In silico studies of the interaction between BRN2 protein and MORE DNA. <i>Journal of Molecular Modeling</i> , 2016, 22, 228.	0.8	3
370	Membrane insertion of a Tc toxin in near-atomic detail. <i>Nature Structural and Molecular Biology</i> , 2016, 23, 884-890.	3.6	88
371	Ureaâ€Aromatic Stacking and Concerted Urea Transport: Conserved Mechanisms in Urea Transporters Revealed by Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5190-5200.	2.3	9
372	Evaluation of Methods for the Calculation of the pK_a of Cysteine Residues in Proteins. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4662-4673.	2.3	88
373	Sulfurâ€Aromatic Interactions: Modeling Cysteine and Methionine Binding to Tyrosinate and Histidinium Ions to Assess Their Influence on Protein Electron Transfer. <i>Israel Journal of Chemistry</i> , 2016, 56, 872-885.	1.0	25
374	Oxidation increases the strength of the methionine-aromatic interaction. <i>Nature Chemical Biology</i> , 2016, 12, 860-866.	3.9	53
375	Specific Binding of Cholesterol to C99 Domain of Amyloid Precursor Protein Depends Critically on Charge State of Protein. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3535-3541.	2.1	35
376	Solvation Thermodynamics of Oligoglycine with Respect to Chain Length and Flexibility. <i>Biophysical Journal</i> , 2016, 111, 756-767.	0.2	12
377	Rotational dynamics of water molecules near biological surfaces with implications for nuclear quadrupole relaxation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24620-24630.	1.3	28
378	Difference in DNA-binding abilities of Fur-homolog DNA binding protein from <i>Neisseria gonorrhoeae</i> . <i>Microbial Pathogenesis</i> , 2016, 99, 62-67.	1.3	0
379	Recent Advances in Computational Models for the Study of Proteinâ€Peptide Interactions. <i>Advances in Protein Chemistry and Structural Biology</i> , 2016, 105, 27-57.	1.0	22
380	Molecular Mechanism of Biased Ligand Conformational Changes in CC Chemokine Receptor 7. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1808-1822.	2.5	13
381	Folding Mechanism of Proteins Im7 and Im9: Insight from All-Atom Simulations in Implicit and Explicit Solvent. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9297-9307.	1.2	12
382	Microscopic Characterization of Membrane Transporter Function by In Silico Modeling and Simulation. <i>Methods in Enzymology</i> , 2016, 578, 373-428.	0.4	8
383	Estimation of Relative Proteinâ€RNA Binding Strengths from Fluctuations in the Bound State. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4593-4599.	2.3	4
384	Effective Riemannian Diffusion Model for Conformational Dynamics of Biomolecular Systems. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4980-4987.	2.1	12

#	ARTICLE	IF	CITATIONS
385	Asymmetric Binding and Metabolism of Polyunsaturated Fatty Acids (PUFAs) by CYP2J2 Epoxygenase. <i>Biochemistry</i> , 2016, 55, 6969-6980.	1.2	30
386	Q-Band Electron-Nuclear Double Resonance Reveals Out-of-Plane Hydrogen Bonds Stabilize an Anionic Ubisemiquinone in Cytochrome bo ₃ from <i>Escherichia coli</i> . <i>Biochemistry</i> , 2016, 55, 5714-5725.	1.2	9
387	Anharmonic Vibrational Analyses of Pentapeptide Conformations Explored with Enhanced Sampling Simulations. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10199-10213.	1.2	11
388	Putative membrane lytic sites of P-type and S-type cardiotoxins from snake venoms as probed by all-atom molecular dynamics simulations. <i>Journal of Molecular Modeling</i> , 2016, 22, 238.	0.8	9
389	Conformational Dynamics on the Extracellular Side of LeuT Controlled by Na ⁺ and K ⁺ Ions and the Protonation State of Glu290. <i>Journal of Biological Chemistry</i> , 2016, 291, 19786-19799.	1.6	22
390	A minimized human insulin-receptor-binding motif revealed in a <i>Conus geographus</i> venom insulin. <i>Nature Structural and Molecular Biology</i> , 2016, 23, 916-920.	3.6	70
391	Practical Aspects of Multiscale Classical and Quantum Simulations of Enzyme Reactions. <i>Methods in Enzymology</i> , 2016, 577, 251-286.	0.4	8
392	Effect of Saturated Very Long-Chain Fatty Acids on the Organization of Lipid Membranes: A Study Combining ² H NMR Spectroscopy and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2016, 120, 6951-6960.	1.2	21
393	Performance of Proteinâ€™Ligand Force Fields for the Flavodoxinâ€™Flavin Mononucleotide System. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3032-3036.	2.1	16
394	Multiscale simulations on conformational dynamics and membrane interactions of the non-structural 2 (NS2) transmembrane domain. <i>Biochemical and Biophysical Research Communications</i> , 2016, 478, 193-198.	1.0	4
395	Identification and Molecular Interaction Studies of Thyroid Hormone Receptor Disruptors among Household Dust Contaminants. <i>Chemical Research in Toxicology</i> , 2016, 29, 1345-1354.	1.7	21
396	Conformational flexibility of the complete catalytic domain of Cdc25B phosphatases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 1567-1575.	1.5	3
397	Binding mode prediction of aplysiatoxin, a potent agonist of protein kinase C, through molecular simulation and structureâ€™activity study on simplified analogs of the receptor-recognition domain. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 4218-4227.	1.4	18
398	Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4534-4548.	2.3	125
399	Further along the Road Less Traveled: AMBER ff15ipq, an Original Protein Force Field Built on a Self-Consistent Physical Model. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3926-3947.	2.3	161
400	Peculiar Aqueous Solubility Trend in Cucurbiturils Unraveled by Atomistic Simulations. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7511-7516.	1.2	11
401	Protein remains stable at unusually high temperatures when solvated in aqueous mixtures of amino acid based ionic liquids. <i>Journal of Molecular Modeling</i> , 2016, 22, 258.	0.8	14
402	A Coiled-Coil Peptide Shaping Lipid Bilayers upon Fusion. <i>Biophysical Journal</i> , 2016, 111, 2162-2175.	0.2	36

#	ARTICLE	IF	CITATIONS
403	A conserved leucine occupies the empty substrate site of LeuT in the Na ⁺ -free return state. <i>Nature Communications</i> , 2016, 7, 11673.	5.8	58
404	An Atomistic View of Amyloidogenic Self-assembly: Structure and Dynamics of Heterogeneous Conformational States in the Pre-nucleation Phase. <i>Scientific Reports</i> , 2016, 6, 33156.	1.6	25
405	Nonlinear backbone torsional pair correlations in proteins. <i>Scientific Reports</i> , 2016, 6, 34481.	1.6	8
406	Acid activation mechanism of the influenza A M2 proton channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E6955-E6964.	3.3	81
407	Crystal Structure of a Full-Length Human Tetraspanin Reveals a Cholesterol-Binding Pocket. <i>Cell</i> , 2016, 167, 1041-1051.e11.	13.5	223
408	Dynamic Conformational States Dictate Selectivity toward the Native Substrate in a Substrate-Permissive Acyltransferase. <i>Biochemistry</i> , 2016, 55, 6314-6326.	1.2	57
409	How Oliceridine (TRV-130) Binds and Stabilizes a μ -Opioid Receptor Conformational State That Selectively Triggers G Protein Signaling Pathways. <i>Biochemistry</i> , 2016, 55, 6456-6466.	1.2	87
410	Protein-Ligand Interaction Detection with a Novel Method of Transient Induced Molecular Electronic Spectroscopy (TIMES): Experimental and Theoretical Studies. <i>ACS Central Science</i> , 2016, 2, 834-842.	5.3	27
411	Structural and functional characterization of a calcium-activated cation channel from <i>Tsukamurella paurometabola</i> . <i>Nature Communications</i> , 2016, 7, 12753.	5.8	11
412	Bilayer Properties of Lipid A from Various Gram-Negative Bacteria. <i>Biophysical Journal</i> , 2016, 111, 1750-1760.	0.2	88
413	Correlation between the number of Pro-Ala repeats in the EmrA homologue of <i>Acinetobacter baumannii</i> and resistance to netilmicin, tobramycin, imipenem and ceftazidime. <i>Journal of Global Antimicrobial Resistance</i> , 2016, 7, 145-149.	0.9	4
414	Simultaneous Optimization of Biomolecular Energy Functions on Features from Small Molecules and Macromolecules. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 6201-6212.	2.3	382
415	Conformational Heterogeneity of Intracellular Loop 3 of the μ -opioid G-protein Coupled Receptor. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11897-11904.	1.2	8
416	QwikMD: Integrative Molecular Dynamics Toolkit for Novices and Experts. <i>Scientific Reports</i> , 2016, 6, 26536.	1.6	153
417	Extended string-like binding of the phosphorylated HP1 N-terminal tail to the lysine 9-methylated histone H3 tail. <i>Scientific Reports</i> , 2016, 6, 22527.	1.6	23
418	Mixed quantum-classical simulations of the vibrational relaxation of photolyzed carbon monoxide in a hemoprotein. <i>Journal of Chemical Physics</i> , 2016, 145, 054108.	1.2	2
419	Simulation Studies of Ion Permeation and Selectivity in Voltage-Gated Sodium Channels. <i>Current Topics in Membranes</i> , 2016, 78, 215-260.	0.5	13
420	Computational analysis of the CB1 carboxyl-terminus in the receptor-G protein complex. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 532-543.	1.5	3

#	ARTICLE	IF	CITATIONS
421	Computational Theory. Springer Theses, 2016, , 31-42.	0.0	0
422	A Discontinuous Potential Model for Protein-Protein Interactions. Molecular Modeling and Simulation, 2016, 2016, 1-20.	0.2	0
423	DNA Scrunching in the Packaging of Viral Genomes. Journal of Physical Chemistry B, 2016, 120, 6200-6207.	1.2	10
424	Silver-Lactoferrin Nanocomplexes as a Potent Antimicrobial Agent. Journal of the American Chemical Society, 2016, 138, 7899-7909.	6.6	73
425	Dynamical Interactions of 5-Fluorouracil Drug with Dendritic Peptide Vectors: The Impact of Dendrimer Generation, Charge, Counterions, and Structured Water. Journal of Physical Chemistry B, 2016, 120, 5732-5743.	1.2	20
426	Insertion of oxidized nucleotide triggers rapid DNA polymerase opening. Nucleic Acids Research, 2016, 44, 4409-4424.	6.5	8
427	Elucidation of Lipid Binding Sites on Lung Surfactant Protein A Using X-ray Crystallography, Mutagenesis, and Molecular Dynamics Simulations. Biochemistry, 2016, 55, 3692-3701.	1.2	25
428	Who's on base? Revealing the catalytic mechanism of inverting family 6 glycoside hydrolases. Chemical Science, 2016, 7, 5955-5968.	3.7	27
429	Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligand-protein interactions. Bioorganic and Medicinal Chemistry, 2016, 24, 4812-4825.	1.4	168
430	Structure-Based Design of 3-(4-Aryl-1 <i>H</i> -1,2,3-triazol-1-yl)-Biphenyl Derivatives as P2Y ₁₄ Receptor Antagonists. Journal of Medicinal Chemistry, 2016, 59, 6149-6168.	2.9	38
431	Conformation Transitions of Recombinant Spidroins via Integration of Time-Resolved FTIR Spectroscopy and Molecular Dynamic Simulation. ACS Biomaterials Science and Engineering, 2016, 2, 1298-1308.	2.6	21
432	Novel protein-inhibitor interactions in site 3 of Ca ²⁺ -bound S100B as discovered by X-ray crystallography. Acta Crystallographica Section D: Structural Biology, 2016, 72, 753-760.	1.1	10
434	Understanding the non-catalytic behavior of human butyrylcholinesterase silent variants: Comparison of wild-type enzyme, catalytically active Ala328Cys mutant, and silent Ala328Asp variant. Chemico-Biological Interactions, 2016, 259, 223-232.	1.7	8
435	Foundations of Molecular Modeling and Simulation. Molecular Modeling and Simulation, 2016, , .	0.2	0
436	Global Rebalancing of Cellular Resources by Pleiotropic Point Mutations Illustrates a Multi-scale Mechanism of Adaptive Evolution. Cell Systems, 2016, 2, 260-271.	2.9	107
438	Modeling structural transitions from the periplasmic-open state of lactose permease and interpretations of spin label experiments. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1541-1552.	1.4	5
439	Balancing Accuracy and Cost of Confinement Simulations by Interpolation and Extrapolation of Confinement Energies. Journal of Chemical Theory and Computation, 2016, 12, 2779-2789.	2.3	5
440	Claws, Disorder, and Conformational Dynamics of the C-Terminal Region of Human Desmoplakin. Journal of Physical Chemistry B, 2016, 120, 8654-8667.	1.2	6

#	ARTICLE	IF	CITATIONS
441	Protein-Backbone Thermodynamics across the Membrane Interface. <i>Journal of Physical Chemistry B</i> , 2016, 120, 6391-6400.	1.2	6
442	A Eukaryotic Sensor for Membrane Lipid Saturation. <i>Molecular Cell</i> , 2016, 63, 49-59.	4.5	108
443	Structure of Penta-Alanine Investigated by Two-Dimensional Infrared Spectroscopy and Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , 2016, 120, 5325-5339.	1.2	18
444	Effective protein model structure refinement by loop modeling and overall relaxation. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 293-301.	1.5	79
445	Conformational Heterogeneity in the Michaelis Complex of Lactate Dehydrogenase: An Analysis of Vibrational Spectroscopy Using Markov and Hidden Markov Models. <i>Journal of Physical Chemistry B</i> , 2016, 120, 6612-6620.	1.2	12
446	Advances in free-energy-based simulations of protein folding and ligand binding. <i>Current Opinion in Structural Biology</i> , 2016, 36, 25-31.	2.6	121
447	An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications. <i>Chemical Reviews</i> , 2016, 116, 4983-5013.	23.0	434
448	Dielectric depolarisation and concerted collective dynamics in AOT reverse micelles with and without ubiquitin. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3606-3617.	1.3	17
449	Simulations of outer membrane channels and their permeability. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 1760-1771.	1.4	44
450	Shock Wave-Induced Damage of a Protein by Void Collapse. <i>Biophysical Journal</i> , 2016, 110, 147-156.	0.2	22
451	Two Na ⁺ Sites Control Conformational Change in a Neurotransmitter Transporter Homolog. <i>Journal of Biological Chemistry</i> , 2016, 291, 1456-1471.	1.6	65
452	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 405-413.	2.3	2,567
453	Improved Parameterization of Amine-Carboxylate and Amine-Phosphate Interactions for Molecular Dynamics Simulations Using the CHARMM and AMBER Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 430-443.	2.3	132
454	An integrated approach with experimental and computational tools outlining the cooperative binding between 2-phenylchromone and human serum albumin. <i>Food Chemistry</i> , 2016, 196, 935-942.	4.2	15
455	Identification of the Glycosaminoglycan Binding Site of Interleukin-10 by NMR Spectroscopy. <i>Journal of Biological Chemistry</i> , 2016, 291, 3100-3113.	1.6	32
456	Effects of phosphorylation on the intrinsic propensity of backbone conformations of serine/threonine. <i>Journal of Biological Physics</i> , 2016, 42, 247-258.	0.7	3
457	Folding of Fibroblast Growth Factor 1 Is Critical for Its Nonclassical Release. <i>Biochemistry</i> , 2016, 55, 1159-1167.	1.2	8
458	Structure-based design of N-substituted 1-hydroxy-4-sulfamoyl-2-naphthoates as selective inhibitors of the Mcl-1 oncoprotein. <i>European Journal of Medicinal Chemistry</i> , 2016, 113, 273-292.	2.6	42

#	ARTICLE	IF	CITATIONS
459	Probing the Salt Concentration Dependent Nucleobase Distribution in a Single-Stranded DNA@Single-Walled Carbon Nanotube Hybrid with Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2016, 120, 455-466.	1.2	25
460	Crystal structures reveal the molecular basis of ion translocation in sodium/proton antiporters. <i>Nature Structural and Molecular Biology</i> , 2016, 23, 248-255.	3.6	83
461	Self-assembled peptides for coating of active sulfur nanoparticles in lithium-sulfur battery. <i>Journal of Nanoparticle Research</i> , 2016, 18, 1.	0.8	10
462	Molecular Insights into the Adsorption Mechanism of Human β -Defensin-3 on Bacterial Membranes. <i>Langmuir</i> , 2016, 32, 1782-1790.	1.6	55
463	Violation of DNA neighbor exclusion principle in RNA recognition. <i>Chemical Science</i> , 2016, 7, 3581-3588.	3.7	17
464	Phosphorylation promotes Al(III) binding to proteins: GECEGSGG as a case study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7197-7207.	1.3	6
465	Determining the Energetics of Small β -Sheet Peptides using Adaptive Steered Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2028-2037.	2.3	22
466	Stability and Function at High Temperature. What Makes a Thermophilic GTPase Different from Its Mesophilic Homologue. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2721-2730.	1.2	20
467	Molecular Basis of S100A1 Activation at Saturating and Subsaturating Calcium Concentrations. <i>Biophysical Journal</i> , 2016, 110, 1052-1063.	0.2	15
468	Novel Inhibitors for a Novel Binding Site in Respiratory Complex III. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2701-2708.	1.2	4
469	Efficient preparation and analysis of membrane and membrane protein systems. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 2468-2482.	1.4	33
470	Conformational Dynamics of the Human Islet Amyloid Polypeptide in a Membrane Environment: Toward the Aggregation Prone Form. <i>Biochemistry</i> , 2016, 55, 2031-2042.	1.2	27
471	Membrane pore formation in atomistic and coarse-grained simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 2266-2277.	1.4	64
472	Coupling between Histone Conformations and DNA Geometry in Nucleosomes on a Microsecond Timescale: Atomistic Insights into Nucleosome Functions. <i>Journal of Molecular Biology</i> , 2016, 428, 221-237.	2.0	131
473	The molecular mechanism of secondary sodium symporters elucidated through the lens of the computational microscope. <i>RSC Advances</i> , 2016, 6, 9522-9540.	1.7	13
474	Importance of Hydrophilic Hydration and Intramolecular Interactions in the Thermodynamics of Helix-Coil Transition and Helix-Helix Assembly in a Deca-Alanine Peptide. <i>Journal of Physical Chemistry B</i> , 2016, 120, 69-76.	1.2	26
475	P-Type ATPases. <i>Methods in Molecular Biology</i> , 2016, , .	0.4	4
476	Coarse-grained bond and angle distributions from atomistic simulations: On the systematic parameterisation of lipid models. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 63, 57-64.	1.3	3

#	ARTICLE	IF	CITATIONS
477	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 281-296.	2.3	2,349
478	A Rigorous and Efficient Method To Reweight Very Large Conformational Ensembles Using Average Experimental Data and To Determine Their Relative Information Content. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 383-394.	2.3	43
479	Synthetic peptide antigens derived from long-chain alpha-neurotoxins: Immunogenicity effect against elapid venoms. <i>Peptides</i> , 2017, 88, 80-86.	1.2	11
480	Highly Coarse-Grained Representations of Transmembrane Proteins. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 935-944.	2.3	17
481	Thermodynamics of Helix-Coil Transitions of Polyalanine in Open Carbon Nanotubes. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 494-499.	2.1	3
482	A Markov State-based Quantitative Kinetic Model of Sodium Release from the Dopamine Transporter. <i>Scientific Reports</i> , 2017, 7, 40076.	1.6	63
483	Structure prediction and network analysis of chitinases from the Cape sundew, <i>Drosera capensis</i> . <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2017, 1861, 636-643.	1.1	13
484	A systematic approach to calibrate a transferable polarizable force field parameter set for primary alcohols. <i>Journal of Computational Chemistry</i> , 2017, 38, 508-517.	1.5	4
485	Sequence-, structure-, and dynamics-based comparisons of structurally homologous CheY-like proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 1578-1583.	3.3	24
486	Molecular Mechanics: Principles, History, and Current Status. , 2017, , 21-67.		2
487	Salt Interactions in Solution Prevent Direct Association of Urea with a Peptide Backbone. <i>Journal of Physical Chemistry B</i> , 2017, 121, 1866-1876.	1.2	12
488	Rigidity and flexibility in the tetrasaccharide linker of proteoglycans from atomic-resolution molecular simulation. <i>Journal of Computational Chemistry</i> , 2017, 38, 1438-1446.	1.5	12
489	Structural basis for nutrient acquisition by dominant members of the human gut microbiota. <i>Nature</i> , 2017, 541, 407-411.	13.7	188
490	Elucidating the Bacterial Membrane Disruption Mechanism of Human α -Defensin 5: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2017, 121, 741-748.	1.2	17
491	Microscopic mechanisms that govern the titration response and p K a values of buried residues in staphylococcal nuclease mutants. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 268-281.	1.5	31
492	Molecular Details of the PH Domain of ACAP1 ^{BAR-PH} Protein Binding to PIP-Containing Membrane. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3586-3596.	1.2	17
493	Extreme biophysics: Enzymes under pressure. <i>Journal of Computational Chemistry</i> , 2017, 38, 1174-1182.	1.5	23
494	Crystal Structure of an LSD-Bound Human Serotonin Receptor. <i>Cell</i> , 2017, 168, 377-389.e12.	13.5	340

#	ARTICLE	IF	CITATIONS
495	Probing the druggability of membrane-bound Rab5 by molecular dynamics simulations. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2017, 32, 434-443.	2.5	14
496	Structural Insights How PIP2 Imposes Preferred Binding Orientations of FAK at Lipid Membranes. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3523-3535.	1.2	28
497	Acetylation dictates the morphology of nanophase biosilica precipitated by a 14-amino acid leucine-lysine peptide. <i>Journal of Peptide Science</i> , 2017, 23, 141-147.	0.8	11
498	STIM1 activates CRAC channels through rotation of the pore helix to open a hydrophobic gate. <i>Nature Communications</i> , 2017, 8, 14512.	5.8	87
499	Conformational dynamics of a neurotransmitter:sodium symporter in a lipid bilayer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E1786-E1795.	3.3	76
500	Deconstruction of the human connexin 26 hemichannel due to an applied electric field; A molecular dynamics simulation study. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 73, 108-114.	1.3	7
501	Computer Simulations of Intrinsically Disordered Proteins. <i>Annual Review of Physical Chemistry</i> , 2017, 68, 117-134.	4.8	68
502	A Partial Calcium-Free Linker Confers Flexibility to Inner-Ear Protocadherin-15. <i>Structure</i> , 2017, 25, 482-495.	1.6	31
503	Grafting Charged Species to Membrane-Embedded Scaffolds Dramatically Increases the Rate of Bilayer Flipping. <i>ACS Central Science</i> , 2017, 3, 186-195.	5.3	16
504	Kinetics of nucleotide entry into RNA polymerase active site provides mechanism for efficiency and fidelity. <i>Biochimica Et Biophysica Acta - Gene Regulatory Mechanisms</i> , 2017, 1860, 482-490.	0.9	12
505	Molecular determinants of the N-terminal acetyltransferase Naa60 anchoring to the Golgi membrane. <i>Journal of Biological Chemistry</i> , 2017, 292, 6821-6837.	1.6	33
506	Newazole derivatives showing antimicrobial effects and their mechanism of antifungal activity by molecular modeling studies. <i>European Journal of Medicinal Chemistry</i> , 2017, 130, 124-138.	2.6	50
507	Gating energetics of a voltage-dependent K^{+} channel pore domain. <i>Journal of Computational Chemistry</i> , 2017, 38, 1472-1478.	1.5	4
508	Computing converged free energy differences between levels of theory via nonequilibrium work methods: Challenges and opportunities. <i>Journal of Computational Chemistry</i> , 2017, 38, 1376-1388.	1.5	28
509	A family 13 thioesterase isolated from an activated sludge metagenome: insights into aromatic compounds metabolism. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1222-1237.	1.5	6
510	Structural properties of amyloid β (1-40) dimer explored by replica exchange molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1024-1045.	1.5	18
511	Insights into proton translocation in cbb 3 oxidase from MD simulations. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2017, 1858, 396-406.	0.5	5
512	Autonomous Generation and Loading of DNA Guides by Bacterial Argonaute. <i>Molecular Cell</i> , 2017, 65, 985-998.e6.	4.5	103

#	ARTICLE	IF	CITATIONS
513	Rapid Estimation of Catalytic Efficiency by Cumulative Atomic Multipole Moments: Application to Ketosteroid Isomerase Mutants. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 945-955.	2.3	9
514	Heterogeneous dielectric generalized Born model with a van der Waals term provides improved association energetics of membrane-embedded transmembrane helices. <i>Journal of Computational Chemistry</i> , 2017, 38, 1308-1320.	1.5	10
515	Simulating the Activation of Voltage Sensing Domain for a Voltage-Gated Sodium Channel Using Polarizable Force Field. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 901-908.	2.1	19
516	Characterization of butyrylcholinesterase in bovine serum. <i>Chemico-Biological Interactions</i> , 2017, 266, 17-27.	1.7	19
517	CryoEM Structure Refinement by Integrating NMR Chemical Shifts with Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3853-3863.	1.2	38
518	1.14*CM1A-LBCC: Localized Bond-Charge Corrected CM1A Charges for Condensed-Phase Simulations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3864-3870.	1.2	413
519	Computational and theoretical advances in studies of intrinsically disordered proteins. <i>Current Opinion in Structural Biology</i> , 2017, 42, 147-154.	2.6	186
520	Single Residue Acts as Gate in Ock Channels. <i>Journal of Physical Chemistry B</i> , 2017, 121, 2614-2621.	1.2	15
521	Conformational Transitions and Alternating-Access Mechanism in the Sarcoplasmic Reticulum Calcium Pump. <i>Journal of Molecular Biology</i> , 2017, 429, 647-666.	2.0	37
522	Electron transfer pathways in a multiheme cytochrome MtrF. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 2916-2921.	3.3	41
523	How Molecular Size Impacts RMSD Applications in Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1518-1524.	2.3	259
524	Palmitoylation of cysteine 415 of CB 1 receptor affects ligand-stimulated internalization and selective interaction with membrane cholesterol and caveolin 1. <i>Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids</i> , 2017, 1862, 523-532.	1.2	24
525	pmx Webserver: A User Friendly Interface for Alchemy. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 109-114.	2.5	50
526	Redox-Driven Conformational Dynamics in a Photosystem-II-Inspired β^2 -Hairpin Maquette Determined through Spectroscopy and Simulation. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3536-3545.	1.2	15
527	Perplexing cooperative folding and stability of a low-sequence complexity, polyproline 2 protein lacking a hydrophobic core. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 2241-2246.	3.3	29
528	Bilayer-Mediated Structural Transitions Control Mechanosensitivity of the TREK-2 K2P Channel. <i>Structure</i> , 2017, 25, 708-718.e2.	1.6	64
529	Optimization of the GBMV2 implicit solvent force field for accurate simulation of protein conformational equilibria. <i>Journal of Computational Chemistry</i> , 2017, 38, 1332-1341.	1.5	24
530	Influence of membrane composition on the binding and folding of a membrane lytic peptide from the non-enveloped flock house virus. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 1190-1199.	1.4	15

#	ARTICLE	IF	CITATIONS
531	Role of Hydrophobic/Aromatic Residues on the Stability of Double-Wall β -Sheet Structures Formed by a Triblock Peptide. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4115-4128.	1.2	5
532	Molecular dynamics simulations of early steps in RNA α -mediated conversion of prions. <i>Protein Science</i> , 2017, 26, 1524-1534.	3.1	11
533	Accelerating physical simulations of proteins by leveraging external knowledge. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2017, 7, e1309.	6.2	16
534	Structural and Functional Analysis of a β ² -Adrenergic Receptor Complex with GRK5. <i>Cell</i> , 2017, 169, 407-421.e16.	13.5	132
535	Full-length, Oligomeric Structure of Wzz Determined by Cryoelectron Microscopy Reveals Insights into Membrane-Bound States. <i>Structure</i> , 2017, 25, 806-815.e3.	1.6	31
536	Molecular Mechanism of Stabilizing the Helical Structure of Huntingtin N17 in a Micellar Environment. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4713-4721.	1.2	11
537	What Can and Cannot Be Learned from Molecular Dynamics Simulations of Bacterial Proton-Coupled Oligopeptide Transporter GkPOT?. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3644-3656.	1.2	27
538	Elongation affinity, activation barrier, and stability of A β ⁴² oligomers/fibrils in physiological saline. <i>Biochemical and Biophysical Research Communications</i> , 2017, 487, 444-449.	1.0	13
539	Size and Origins of Long-Range Orientational Water Correlations in Dilute Aqueous Salt Solutions. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2031-2035.	2.1	22
540	Mapping the conformational free energy of aspartic acid in the gas phase and in aqueous solution. <i>Journal of Chemical Physics</i> , 2017, 146, 145102.	1.2	10
541	cDNA cloning, molecular modeling and docking calculations of L-type lectins from <i>Swartzia simplex</i> var. <i>grandiflora</i> (Leguminosae, Papilionoideae), a member of the tribe Swartzieae. <i>Phytochemistry</i> , 2017, 139, 60-71.	1.4	6
542	Toward the rational design of macrolide antibiotics to combat resistance. <i>Chemical Biology and Drug Design</i> , 2017, 90, 641-652.	1.5	10
543	Discrimination of Native-like States of Membrane Proteins with Implicit Membrane-based Scoring Functions. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3049-3059.	2.3	6
544	CHARMM-GUI ligand reader and modeler for CHARMM force field generation of small molecules. <i>Journal of Computational Chemistry</i> , 2017, 38, 1879-1886.	1.5	311
545	Unidirectional Transport Mechanism in an ATP Dependent Exporter. <i>ACS Central Science</i> , 2017, 3, 250-258.	5.3	19
546	Molecular interactions between tubulin tails and glutamylases reveal determinants of glutamylation patterns. <i>EMBO Reports</i> , 2017, 18, 1013-1026.	2.0	27
547	Perturbation α Response Scanning Reveals Key Residues for Allosteric Control in Hsp70. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1359-1374.	2.5	70
548	Effects of Hydrotropic Salt on the Nanoscopic Dynamics of DTAB Micelles. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5562-5572.	1.2	19

#	ARTICLE	IF	CITATIONS
549	Identification and Characterization of a Secondary Sodium-Binding Site and the Main Selectivity Determinants in the Human Concentrative Nucleoside Transporter 3. <i>Molecular Pharmaceutics</i> , 2017, 14, 1980-1987.	2.3	10
550	Comparative molecular dynamics study of neuromyelitis optica-immunoglobulin G binding to aquaporin-4 extracellular domains. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 1326-1334.	1.4	9
551	Neural Network and Nearest Neighbor Algorithms for Enhancing Sampling of Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2489-2500.	2.3	51
552	Simulated Force Quench Dynamics Shows GB1 Protein Is Not a Two State Folder. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5162-5173.	1.2	14
553	Parameter Optimization for Interaction between C-Terminal Domains of HIV-1 Capsid Protein. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1134-1141.	2.5	3
554	On the permeation of large organic cations through the pore of ATP-gated P2X receptors. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E3786-E3795.	3.3	79
555	LigParGen web server: an automatic OPLS-AA parameter generator for organic ligands. <i>Nucleic Acids Research</i> , 2017, 45, W331-W336.	6.5	829
556	The Isomeric Preference of an Atypical Dopamine Transporter Inhibitor Contributes to Its Selection of the Transporter Conformation. <i>ACS Chemical Neuroscience</i> , 2017, 8, 1735-1746.	1.7	31
557	Electronic absorption spectra of pyridine and nicotine in aqueous solution with a combined molecular dynamics and polarizable QM/MM approach. <i>Journal of Computational Chemistry</i> , 2017, 38, 319-335.	1.5	38
558	Desulfination by 2-hydroxybiphenyl-2-sulfinate desulfinase proceeds via electrophilic aromatic substitution by the cysteine-27 proton. <i>Chemical Science</i> , 2017, 8, 5078-5086.	3.7	9
559	A multiscale computational modelling approach predicts mechanisms of female sex risk in the setting of arousal-induced arrhythmias. <i>Journal of Physiology</i> , 2017, 595, 4695-4723.	1.3	41
560	The role of the Met20 loop in the hydride transfer in <i>Escherichia coli</i> dihydrofolate reductase. <i>Journal of Biological Chemistry</i> , 2017, 292, 14229-14239.	1.6	24
561	Architecture of the paracellular channels formed by claudins of the blood-brain barrier tight junctions. <i>Annals of the New York Academy of Sciences</i> , 2017, 1405, 131-146.	1.8	56
562	Structural Mimicry of the Dengue Virus Envelope Glycoprotein Revealed by the Crystallographic Study of an Idiotypic Anti-idiotypic Fab Complex. <i>Journal of Virology</i> , 2017, 91, .	1.5	6
563	A new class of enhanced kinetic sampling methods for building Markov state models. <i>Journal of Chemical Physics</i> , 2017, 147, 152702.	1.2	14
564	Hotspots of age-related protein degradation: the importance of neighboring residues for the formation of non-disulfide crosslinks derived from cysteine. <i>Biochemical Journal</i> , 2017, 474, 2475-2487.	1.7	15
565	Probing the disparate effects of arginine and lysine residues on antimicrobial peptide/bilayer association. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 1941-1950.	1.4	35
566	Gibbs Sampler-Based $\hat{\mu}$ -Dynamics and Rao-Blackwell Estimator for Alchemical Free Energy Calculation. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2501-2510.	2.3	33

#	ARTICLE	IF	CITATIONS
567	Monomeric Polyglutamine Structures That Evolve into Fibrils. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5953-5967.	1.2	18
568	Amino Acid Interaction (INTAA) web server. <i>Nucleic Acids Research</i> , 2017, 45, W388-W392.	6.5	38
569	Synthesis, antiviral evaluation and molecular docking studies of N4-aryl substituted/unsubstituted thiosemicarbazones derived from 1-indanones as potent anti-bovine viral diarrhea virus agents. <i>Bioorganic and Medicinal Chemistry</i> , 2017, 25, 4055-4063.	1.4	24
570	Structural Properties of Nonionic Monorhamnolipid Aggregates in Water Studied by Classical Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5781-5793.	1.2	23
571	Structural review of PPAR α in complex with ligands: Cartesian- and dihedral angle principal component analyses of X-ray crystallographic data. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1684-1698.	1.5	5
572	Probing the dynamics of disorder. <i>Progress in Biophysics and Molecular Biology</i> , 2017, 128, 57-62.	1.4	2
573	Predicting the orientation of protein G B1 on hydrophobic surfaces using Monte Carlo simulations. <i>Biointerphases</i> , 2017, 12, 02D401.	0.6	23
574	Molecular dynamics simulations reveal the conformational dynamics of Arabidopsis thaliana BRI1 and BAK1 receptor-like kinases. <i>Journal of Biological Chemistry</i> , 2017, 292, 12643-12652.	1.6	45
575	Molecular dynamics simulation of the nanofibrils formed by amyloid-based peptide amphiphiles. <i>Molecular Simulation</i> , 2017, 43, 1227-1239.	0.9	4
576	Structural and functional effects of nucleotide variation on the human TB drug metabolizing enzyme arylamine N -acetyltransferase 1. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 75, 330-339.	1.3	13
577	Elucidating Surface Ligand-Dependent Kinetic Enhancement of Proteolytic Activity at Surface-Modified Quantum Dots. <i>ACS Nano</i> , 2017, 11, 5884-5896.	7.3	39
578	Metadynamic metainference: Convergence towards force field independent structural ensembles of a disordered peptide. <i>Journal of Chemical Physics</i> , 2017, 146, 165102.	1.2	47
579	Ion-pulling simulations provide insights into the mechanisms of channel opening of the skeletal muscle ryanodine receptor. <i>Journal of Biological Chemistry</i> , 2017, 292, 12947-12958.	1.6	11
580	pH Sensing Properties of Flexible, Bias-Free Graphene Microelectrodes in Complex Fluids: From Phosphate Buffer Solution to Human Serum. <i>Small</i> , 2017, 13, 1700564.	5.2	5
581	Inclusion of lipopeptides into the DMPC lipid bilayers prevents A β peptide insertion. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10087-10098.	1.3	6
582	Modulating short tryptophan- and arginine-rich peptides activity by substitution with histidine. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2017, 1861, 1844-1854.	1.1	31
583	Rational Design of New Antimicrobial Peptides Targeting Gram Negative Bacteria. <i>Biophysical Journal</i> , 2017, 112, 386a.	0.2	1
584	Systematic Parameterization of Lignin for the Charmm Force Field. <i>Biophysical Journal</i> , 2017, 112, 449a.	0.2	0

#	ARTICLE	IF	CITATIONS
585	Mechanism of Substrate Translocation in an Alternating Access Transporter. <i>Cell</i> , 2017, 169, 96-107.e12.	13.5	89
586	<i>Yersinia</i> effector protein (YopO)-mediated phosphorylation of host gelsolin causes calcium-independent activation leading to disruption of actin dynamics. <i>Journal of Biological Chemistry</i> , 2017, 292, 8092-8100.	1.6	13
587	Binding mode analyses of NAP derivatives as mu opioid receptor selective ligands through docking studies and molecular dynamics simulation. <i>Bioorganic and Medicinal Chemistry</i> , 2017, 25, 2463-2471.	1.4	11
588	Structural basis for selectivity and diversity in angiotensin II receptors. <i>Nature</i> , 2017, 544, 327-332.	13.7	174
589	Polarizable charge equilibration model for predicting accurate electrostatic interactions in molecules and solids. <i>Journal of Chemical Physics</i> , 2017, 146, 124117.	1.2	43
590	Radiolabeled Dibenzodiazepinone-Type Antagonists Give Evidence of Dualsteric Binding at the M ₂ Muscarinic Acetylcholine Receptor. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 3314-3334.	2.9	25
591	Novel de novo variant in <i>EBF3</i> is likely to impact DNA binding in a patient with a neurodevelopmental disorder and expanded phenotypes: patient report, in silico functional assessment, and review of published cases. <i>Journal of Physical Education and Sports Management</i> , 2017, 3, a001743.	0.5	22
592	Critical Comparison of Biomembrane Force Fields: Protein-Lipid Interactions at the Membrane Interface. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2310-2321.	2.3	62
593	Preexisting domain motions underlie protonation-dependent structural transitions of the P-type Ca ²⁺ -ATPase. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10153-10162.	1.3	11
594	Computational protein structure refinement: almost there, yet still so far to go. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2017, 7, e1307.	6.2	57
595	Computer simulations of the diffusion of Na ⁺ and Cl ⁻ ions across POPC lipid bilayer membranes. <i>Journal of Chemical Physics</i> , 2017, 146, 105101.	1.2	6
596	Structures of closed and open states of a voltage-gated sodium channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E3051-E3060.	3.3	139
597	Thermodynamics of Protein Folding Studied by Umbrella Sampling along a Reaction Coordinate of Native Contacts. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2086-2097.	2.3	20
598	Understanding the interfacial behavior of lysozyme on Au (111) surfaces with multiscale simulations. <i>Applied Physics Letters</i> , 2017, 110, .	1.5	9
599	Extension of the Highly Mobile Membrane Mimetic to Transmembrane Systems through Customized <i>in Silico</i> Solvents. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3764-3776.	1.2	19
600	Molecular dynamics simulations and molecular flooding studies of the retinoid X-receptor ligand binding domain. <i>Journal of Molecular Modeling</i> , 2017, 23, 98.	0.8	12
601	Atomistic Study of Intramolecular Interactions in the Closed-State Channelrhodopsin Chimera, C1C2. <i>Biophysical Journal</i> , 2017, 112, 943-952.	0.2	17
602	Reparametrization of Protein Force Field Nonbonded Interactions Guided by Osmotic Coefficient Measurements from Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1812-1826.	2.3	37

#	ARTICLE	IF	CITATIONS
603	Novel Noncatalytic Substrate-Selective p38 β -Specific MAPK Inhibitors with Endothelial-Stabilizing and Anti-Inflammatory Activity. <i>Journal of Immunology</i> , 2017, 198, 3296-3306.	0.4	31
604	Nanoindentation of a new graphene/phospholipid composite: a numerical simulation. , 2017, , .		1
605	Docking, molecular dynamics and free energy studies on aspartoacylase mutations involved in Canavan disease. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 74, 44-53.	1.3	14
606	Determinants of Alanine Dipeptide Conformational Equilibria on Graphene and Hydroxylated Derivatives. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3895-3907.	1.2	23
607	Identification of novel serotonin reuptake inhibitors targeting central and allosteric binding sites: A virtual screening and molecular dynamics simulations study. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 74, 193-202.	1.3	8
608	Molecular dynamics simulation of the atomistic monolayer structures of N-acyl amino acid-based surfactants. <i>Molecular Simulation</i> , 2017, 43, 491-501.	0.9	44
609	Reactive Center Loop Insertion in β -1-Antitrypsin Captured by Accelerated Molecular Dynamics Simulation. <i>Biochemistry</i> , 2017, 56, 634-646.	1.2	20
610	A QM/MM study of the nature of the entatic state in plastocyanin. <i>Journal of Computational Chemistry</i> , 2017, 38, 1431-1437.	1.5	16
611	Model of the Interaction between the NF- κ B Inhibitory Protein p100 and the E3 Ubiquitin Ligase β -TrCP based on NMR and Docking Experiments. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 223-233.	2.5	7
612	Computing the binding affinity of a ligand buried deep inside a protein with the hybrid steered molecular dynamics. <i>Biochemical and Biophysical Research Communications</i> , 2017, 483, 203-208.	1.0	15
613	Understanding the Phosphorylation Mechanism by Using Quantum Chemical Calculations and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3565-3573.	1.2	12
614	Differential Membrane Binding Mechanics of Synaptotagmin Isoforms Observed in Atomic Detail. <i>Biochemistry</i> , 2017, 56, 281-293.	1.2	39
615	A computational approach for studying antibody-antigen interactions without prior structural information: the anti-testosterone binding antibody as a case study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 322-331.	1.5	4
616	Investigation of the Effect of Bilayer Composition on PKC β -C2 Domain Docking Using Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 78-88.	1.2	18
617	Revised RNA Dihedral Parameters for the Amber Force Field Improve RNA Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 900-915.	2.3	103
618	Toward Understanding the Structural Basis of Partial Agonism at the Dopamine D ₃ Receptor. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 580-593.	2.9	49
619	Toward amino acid typing for proteins in FFLUX. <i>Journal of Computational Chemistry</i> , 2017, 38, 336-345.	1.5	12
620	Molecular insights into the enzyme promiscuity of an aromatic prenyltransferase. <i>Nature Chemical Biology</i> , 2017, 13, 226-234.	3.9	100

#	ARTICLE	IF	CITATIONS
621	Finite Temperature String Method with Umbrella Sampling: Application on a Side Chain Flipping in Mhp1 Transporter. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3376-3386.	1.2	14
622	Norovirus Escape from Broadly Neutralizing Antibodies Is Limited to Allosteric-Like Mechanisms. <i>MSphere</i> , 2017, 2, .	1.3	30
623	Structural, physicochemical and dynamic features conserved within the aerolysin pore-forming toxin family. <i>Scientific Reports</i> , 2017, 7, 13932.	1.6	38
624	Structural and mechanistic insights into the biosynthesis of CDP-archaeol in membranes. <i>Cell Research</i> , 2017, 27, 1378-1391.	5.7	10
625	Understanding the differences of the ligand binding/unbinding pathways between phosphorylated and non-phosphorylated ARH1 using molecular dynamics simulations. <i>Scientific Reports</i> , 2017, 7, 12439.	1.6	21
626	Chemical substitutions in the selectivity filter of potassium channels do not rule out constricted-like conformations for C-type inactivation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 11145-11150.	3.3	29
627	Assessing the Structure and Stability of Transmembrane Oligomeric Intermediates of an Î±-Helical Toxin. <i>Langmuir</i> , 2017, 33, 11496-11510.	1.6	25
628	Role of Ureaâ€™s Aromatic Stacking Interactions in Stabilizing the Aromatic Residues of the Protein in Urea-Induced Denatured State. <i>Journal of the American Chemical Society</i> , 2017, 139, 14931-14946.	6.6	47
629	Chasing the open-state structure of pentameric ligand-gated ion channels. <i>Journal of General Physiology</i> , 2017, 149, 1119-1138.	0.9	33
630	Mechanistic principles underlying regulation of the actin cytoskeleton by phosphoinositides. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E8977-E8986.	3.3	106
631	Sequence-Dependent Interfacial Adsorption and Permeation of Dipeptides across Phospholipid Membranes. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9859-9867.	1.2	8
632	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.	2.3	29
633	Phosphatidylinositol (4, 5)-bisphosphate targets double C2 domain protein B to the plasma membrane. <i>Traffic</i> , 2017, 18, 825-839.	1.3	15
634	Predictions for Î±-Helical Glycopeptide Design from Structural Bioinformatics Analysis. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2598-2611.	2.5	2
635	Affinity and path of binding xylopyranose unto E.Â‘coli xylose permease. <i>Biochemical and Biophysical Research Communications</i> , 2017, 494, 202-206.	1.0	10
636	Toward Understanding Mcl-1 Promiscuous and Specific Binding Mode. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2885-2895.	2.5	13
637	New generation of docking programs: Supercomputer validation of force fields and quantum-chemical methods for docking. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 78, 139-147.	1.3	37
638	Simulations of a Graphene Nanoflake as a Nanovector To Improve ZnPc Phototherapy Toxicity: From Vacuum to Cell Membrane. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 37554-37562.	4.0	20

#	ARTICLE	IF	CITATIONS
639	Examining the role of protein structural dynamics in drug resistance in <i>Mycobacterium tuberculosis</i> . <i>Chemical Science</i> , 2017, 8, 8384-8399.	3.7	19
640	Rare ADAR and RNASEH2B variants and a type I interferon signature in glioma and prostate carcinoma risk and tumorigenesis. <i>Acta Neuropathologica</i> , 2017, 134, 905-922.	3.9	12
641	Molecular Simulations of Melittin-Induced Membrane Pores. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10209-10214.	1.2	27
642	Photochemical Identification of Molecular Binding Sites on the Surface of Amyloid- β Fibrillar Aggregates. <i>CheM</i> , 2017, 3, 898-912.	5.8	27
643	The Conformational Change in Elongation Factor Tu Involves Separation of Its Domains. <i>Biochemistry</i> , 2017, 56, 5972-5979.	1.2	12
644	Molecular dynamics simulations of heterogeneous cell membranes in response to uniaxial membrane stretches at high loading rates. <i>Scientific Reports</i> , 2017, 7, 8316.	1.6	14
645	Development of novel biosensors to study receptor-mediated activation of the G-protein $\beta\gamma$ subunits Gs and Golf. <i>Journal of Biological Chemistry</i> , 2017, 292, 19989-19998.	1.6	14
646	D ₄ dopamine receptor high-resolution structures enable the discovery of selective agonists. <i>Science</i> , 2017, 358, 381-386.	6.0	176
647	QM/MM Study of the Nitrogenase MoFe Protein Resting State: Broken-Symmetry States, Protonation States, and QM Region Convergence in the FeMoco Active Site. <i>Inorganic Chemistry</i> , 2017, 56, 13417-13429.	1.9	74
648	Computational Model and Dynamics of Monomeric Full-Length APOBEC3G. <i>ACS Central Science</i> , 2017, 3, 1180-1188.	5.3	32
649	Effect of the solvent on the conformational behavior of the alanine dipeptide deduced from MD simulations. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 78, 118-128.	1.3	14
650	Conversion of OprO into an OprP-like Channel by Exchanging Key Residues in the Channel Constriction. <i>Biophysical Journal</i> , 2017, 113, 829-834.	0.2	10
651	Picomolar Fingerprinting of Nucleic Acid Nanoparticles Using Solid-State Nanopores. <i>ACS Nano</i> , 2017, 11, 9701-9710.	7.3	54
652	Two transmembrane dimers of the bovine papillomavirus E5 oncoprotein clamp the PDGF β receptor in an active dimeric conformation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E7262-E7271.	3.3	26
653	Tracking Dehydration Mechanisms in Crystalline Hydrates with Molecular Dynamics Simulations. <i>Crystal Growth and Design</i> , 2017, 17, 5017-5022.	1.4	25
654	Glycans—Tools for Preparing Carbohydrate Structures for Atomistic Simulations of Glycoproteins, Glycolipids, and Carbohydrate Polymers for GROMACS. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2401-2406.	2.5	71
655	CryoEM structure of MxB reveals a novel oligomerization interface critical for HIV restriction. <i>Science Advances</i> , 2017, 3, e1701264.	4.7	47
656	Pyrophosphate Release in the Protein HIV Reverse Transcriptase. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9557-9565.	1.2	15

#	ARTICLE	IF	CITATIONS
657	Two novel mutations in ZAP70 gene that result in human immunodeficiency. <i>Clinical Immunology</i> , 2017, 183, 278-284.	1.4	9
658	Non-local effects of point mutations on the stability of a protein module. <i>Journal of Chemical Physics</i> , 2017, 147, 105101.	1.2	6
659	Asymmetric mechanosensitivity in a eukaryotic ion channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E8343-E8351.	3.3	45
660	Microsecond Dynamics and Network Analysis of the HIV-1 SOSIP Env Trimer Reveal Collective Behavior and Conserved Microdomains of the Glycan Shield. <i>Structure</i> , 2017, 25, 1631-1639.e2.	1.6	42
661	Peptides derived from transcription factor EB bind to calcineurin at a similar region as the NFAT-type motif. <i>Biochimie</i> , 2017, 142, 158-167.	1.3	10
662	Binding and Release between Polymeric Carrier and Protein Drug: pH-Mediated Interplay of Coulomb Forces, Hydrogen Bonding, van der Waals Interactions, and Entropy. <i>Biomacromolecules</i> , 2017, 18, 3665-3677.	2.6	15
663	Towards a complete characterization of the $\hat{\Gamma}$ -dispersion in dielectric spectroscopy of protein-water systems. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 26980-26985.	1.3	23
664	Dynamic and Kinetic Elements of $\hat{\mu}$ -Opioid Receptor Functional Selectivity. <i>Scientific Reports</i> , 2017, 7, 11255.	1.6	44
665	Discovery of Inhibitors of Four Bromodomains by Fragment-Anchored Ligand Docking. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2584-2597.	2.5	21
666	Structure and Dynamics of FosA-Mediated Fosfomycin Resistance in <i>Klebsiella pneumoniae</i> and <i>Escherichia coli</i> . <i>Antimicrobial Agents and Chemotherapy</i> , 2017, 61, .	1.4	28
667	Co-operative intra-protein structural response due to protein-protein complexation revealed through thermodynamic quantification: study of MDM2-p53 binding. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 891-903.	1.3	3
668	Hydration properties of the polyanines by atomistic molecular dynamics. <i>Journal of Molecular Liquids</i> , 2017, 244, 285-290.	2.3	6
669	pH-mediated gating and formate transport mechanism in the <i>Escherichia coli</i> formate channel. <i>Molecular Simulation</i> , 2017, 43, 1300-1306.	0.9	3
670	Physical properties of the HIV-1 capsid from all-atom molecular dynamics simulations. <i>Nature Communications</i> , 2017, 8, 15959.	5.8	136
671	Dynamic role of the tether helix in PIP2-dependent gating of a G protein-gated potassium channel. <i>Journal of General Physiology</i> , 2017, 149, 799-811.	0.9	35
672	Assessing the interaction between surfactant-like peptides and lipid membranes. <i>RSC Advances</i> , 2017, 7, 35973-35981.	1.7	22
673	Structural, mutagenic and <i>in silico</i> studies of xyloglucan fucosylation in <i>Arabidopsis thaliana</i> suggest a water-mediated mechanism. <i>Plant Journal</i> , 2017, 91, 931-949.	2.8	53
674	Evaluating amber force fields using computed NMR chemical shifts. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1944-1956.	1.5	9

#	ARTICLE	IF	CITATIONS
675	Evolution of Aggregate Structure in Solutions of Anionic Monorhamnolipids: Experimental and Computational Results. <i>Langmuir</i> , 2017, 33, 7412-7424.	1.6	27
676	Death Receptor 5 Activation Is Energetically Coupled to Opening of the Transmembrane Domain Dimer. <i>Biophysical Journal</i> , 2017, 113, 381-392.	0.2	9
677	Residue Specific Interaction of an Unfolded Protein with Solvents in Mixed Water/Ethanol Solutions: A Combined Molecular Dynamics and ONIOM Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6172-6186.	1.1	6
678	Role of the disulfide bond in stabilizing and folding of the fimbrial protein DraE from uropathogenic <i>Escherichia coli</i> . <i>Journal of Biological Chemistry</i> , 2017, 292, 16136-16149.	1.6	9
679	Molecular dynamics of conformation-specific dopamine transporter-inhibitor complexes. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 76, 143-151.	1.3	5
680	Conformational Transitions of the Pituitary Adenylate Cyclase-Activating Polypeptide Receptor, a Human Class B GPCR. <i>Scientific Reports</i> , 2017, 7, 5427.	1.6	19
681	Insights into the <i>Giardia intestinalis</i> enolase and human plasminogen interaction. <i>Molecular BioSystems</i> , 2017, 13, 2015-2023.	2.9	9
682	GENESIS 1.1: A hybrid-parallel molecular dynamics simulator with enhanced sampling algorithms on multiple computational platforms. <i>Journal of Computational Chemistry</i> , 2017, 38, 2193-2206.	1.5	133
683	A polar SxxS motif drives assembly of the transmembrane domains of Toll-like receptor 4. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 2086-2095.	1.4	12
684	Structural basis for substrate selection by the translocation and assembly module of the β -barrel assembly machinery. <i>Molecular Microbiology</i> , 2017, 106, 142-156.	1.2	29
685	Simulation of Ligand Binding to Membrane Proteins. <i>Methods in Molecular Biology</i> , 2017, 1635, 359-381.	0.4	5
686	Characterization of long and stable de novo single alpha-helix domains provides novel insight into their stability. <i>Scientific Reports</i> , 2017, 7, 44341.	1.6	40
687	The length but not the sequence of peptide linker modules exerts the primary influence on the conformations of protein domains in cellulosome multi-enzyme complexes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21414-21425.	1.3	17
688	An optimal distance cutoff for contact-based Protein Structure Networks using side-chain centers of mass. <i>Scientific Reports</i> , 2017, 7, 2838.	1.6	70
689	Exploring the binding sites and proton diffusion on insulin amyloid fibril surfaces by naphthol-based photoacid fluorescence and molecular simulations. <i>Scientific Reports</i> , 2017, 7, 6245.	1.6	17
690	Engineered isopeptide bond stabilized fibrin inspired nanoscale peptide based sealants for efficient blood clotting. <i>Scientific Reports</i> , 2017, 7, 6509.	1.6	5
691	A novel proton transfer mechanism in the SLC11 family of divalent metal ion transporters. <i>Scientific Reports</i> , 2017, 7, 6194.	1.6	29
692	In silico model of the human ClC-Kb chloride channel: pore mapping, biostructural pathology and drug screening. <i>Scientific Reports</i> , 2017, 7, 7249.	1.6	15

#	ARTICLE	IF	CITATIONS
693	The Surface of Protein α 85 Can Act as a Template for Recurring Poly(ethylene glycol) Structure. <i>Biochemistry</i> , 2017, 56, 5671-5678.	1.2	12
695	Molecular dynamics of the cryo-EM CFTR structure. <i>Biochemical and Biophysical Research Communications</i> , 2017, 491, 986-993.	1.0	14
696	α -Glucosidase inhibitory effect of <i>Potentilla astracanica</i> and some isoflavones: Inhibition kinetics and mechanistic insights through in vitro and in silico studies. <i>International Journal of Biological Macromolecules</i> , 2017, 105, 1062-1070.	3.6	58
697	Intramolecular Interactions Overcome Hydration to Drive the Collapse Transition of Gly ₁₅ . <i>Journal of Physical Chemistry B</i> , 2017, 121, 8078-8084.	1.2	26
698	Role of Electrostatics in Protein-RNA Binding: The Global vs the Local Energy Landscape. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8437-8446.	1.2	20
699	Prediction of Reduction Potentials of Copper Proteins with Continuum Electrostatics and Density Functional Theory. <i>Chemistry - A European Journal</i> , 2017, 23, 15436-15445.	1.7	20
700	Mechanism of intracellular allosteric β 2AR antagonist revealed by X-ray crystal structure. <i>Nature</i> , 2017, 548, 480-484.	13.7	148
701	The sensitivity of folding free energy landscapes of trpzips to mutations in the hydrophobic core. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 22813-22825.	1.3	5
702	Asymmetric breathing motions of nucleosomal DNA and the role of histone tails. <i>Journal of Chemical Physics</i> , 2017, 147, 065101.	1.2	14
703	Hormesis of some organic solvents on <i>Vibrio qinghaiensis</i> sp.-Q67 from first binding to the β 2 subunit of luciferase. <i>RSC Advances</i> , 2017, 7, 37636-37642.	1.7	12
704	Coexisting origins of subdiffusion in internal dynamics of proteins. <i>Physical Review E</i> , 2017, 95, 062403.	0.8	13
705	Ketamine Inhibition of the Pentameric Ligand-Gated Ion Channel GLIC. <i>Biophysical Journal</i> , 2017, 113, 605-612.	0.2	4
706	Allosteric pyruvate kinase-based α -logic gate synergistically senses energy and sugar levels in <i>Mycobacterium tuberculosis</i> . <i>Nature Communications</i> , 2017, 8, 1986.	5.8	49
707	Allosteric Control of a Plant Receptor Kinase through S-Glutathionylation. <i>Biophysical Journal</i> , 2017, 113, 2354-2363.	0.2	47
708	Identification of Two New Cholesterol Interaction Sites on the A2A Adenosine Receptor. <i>Biophysical Journal</i> , 2017, 113, 2415-2424.	0.2	61
709	Identification of the functional states of human vitamin K epoxide reductase from molecular dynamics simulations. <i>RSC Advances</i> , 2017, 7, 52071-52090.	1.7	10
710	Demystifying P2Y ₁ Receptor Ligand Recognition through Docking and Molecular Dynamics Analyses. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 3104-3123.	2.5	20
711	Elucidating the stability of bolaamphiphilic polypeptide nanosheets using atomistic molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31921-31928.	1.3	26

#	ARTICLE	IF	CITATIONS
712	Evaluating Force-Field London Dispersion Coefficients Using the Exchange-Hole Dipole Moment Model. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6146-6157.	2.3	40
713	Iodide Binding in Sodium-Coupled Cotransporters. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 3043-3055.	2.5	12
714	Parameterization of Palmitoylated Cysteine, Farnesylated Cysteine, Geranylgeranylated Cysteine, and Myristoylated Glycine for the Martini Force Field. <i>Journal of Physical Chemistry B</i> , 2017, 121, 11132-11143.	1.2	33
715	Structure of FlgK reveals the divergence of the bacterial Hook-Filament Junction of <i>Campylobacter</i> . <i>Scientific Reports</i> , 2017, 7, 15743.	1.6	11
716	Slow-Down in Diffusion in Crowded Protein Solutions Correlates with Transient Cluster Formation. <i>Journal of Physical Chemistry B</i> , 2017, 121, 11072-11084.	1.2	93
717	Hydration peculiarities of graphene oxides with multiple oxidation degrees. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32333-32340.	1.3	21
718	Structure and Misfolding of the Flexible Tripartite Coiled-Coil Domain of Glaucoma-Associated Myocilin. <i>Structure</i> , 2017, 25, 1697-1707.e5.	1.6	26
719	Can Relative Binding Free Energy Predict Selectivity of Reversible Covalent Inhibitors?. <i>Journal of the American Chemical Society</i> , 2017, 139, 17945-17952.	6.6	44
720	Origin of the omnipotence of eukaryotic release factor 1. <i>Nature Communications</i> , 2017, 8, 1425.	5.8	15
721	PLA2-like proteins myotoxic mechanism: a dynamic model description. <i>Scientific Reports</i> , 2017, 7, 15514.	1.6	31
722	Correlating kinetic and structural data on ubiquinone binding and reduction by respiratory complex I. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 12737-12742.	3.3	91
723	Physical driving force of actomyosin motility based on the hydration effect. <i>Cytoskeleton</i> , 2017, 74, 512-527.	1.0	9
724	Cholesterol Promotes Protein Binding by Affecting Membrane Electrostatics and Solvation Properties. <i>Biophysical Journal</i> , 2017, 113, 2004-2015.	0.2	38
725	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5933-5944.	2.3	139
726	Two-Step Adsorption of PtCl ₆ ²⁻ Complexes at a Charged Langmuir Monolayer: Role of Hydration and Ion Correlations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25377-25383.	1.5	28
727	Rose Bengal Binding to Collagen and Tissue Photobonding. <i>ACS Omega</i> , 2017, 2, 6646-6657.	1.6	41
728	Effect of amino acid mutations on intra-dimer tubulin-tubulin binding strength of microtubules. <i>Integrative Biology (United Kingdom)</i> , 2017, 9, 925-933.	0.6	1
729	Structural predictions for curli amyloid fibril subunits CsgA and CsgB. <i>RSC Advances</i> , 2017, 7, 48102-48112.	1.7	35

#	ARTICLE	IF	CITATIONS
730	â€œMartinizingâ€ the Variational Implicit Solvent Method (VISM): Solvation Free Energy for Coarse-Grained Proteins. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6538-6548.	1.2	10
731	Critical Role of Water Molecules in Proton Translocation by the Membrane-Bound Transhydrogenase. <i>Structure</i> , 2017, 25, 1111-1119.e3.	1.6	12
732	Cation solvation with quantum chemical effects modeled by a size-consistent multi-partitioning quantum mechanics/molecular mechanics method. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17985-17997.	1.3	10
733	On the role of subunit M in cytochrome cbb 3 oxidase. <i>Biochemical and Biophysical Research Communications</i> , 2017, 491, 47-52.	1.0	1
734	Atomic resolution conformational dynamics of intrinsically disordered proteins from NMR spin relaxation. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2017, 102-103, 43-60.	3.9	43
735	Evaluating Force Field Performance in Thermodynamic Calculations of Cyclodextrin Hostâ€™Guest Binding: Water Models, Partial Charges, and Host Force Field Parameters. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4253-4269.	2.3	51
736	Advancing Drug Discovery through Enhanced Free Energy Calculations. <i>Accounts of Chemical Research</i> , 2017, 50, 1625-1632.	7.6	211
737	Activation of the Unfolded Protein Response by Lipid Bilayer Stress. <i>Molecular Cell</i> , 2017, 67, 673-684.e8.	4.5	252
738	Molecular Chains Interacting by Lennard-Jones and Coulomb Forces. <i>Qualitative Theory of Dynamical Systems</i> , 2017, 16, 591-608.	0.8	3
739	Significantly Improved Protein Folding Thermodynamics Using a Dispersion-Corrected Water Model and a New Residue-Specific Force Field. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3199-3205.	2.1	33
740	Mutations in human AID differentially affect its ability to deaminate cytidine and 5-methylcytidine in ssDNA substrates in vitro. <i>Scientific Reports</i> , 2017, 7, 3873.	1.6	7
741	Molecular Dynamics Simulation Reveals Unique Interplays Between a Tarantula Toxin and Lipid Membranes. <i>Journal of Membrane Biology</i> , 2017, 250, 315-325.	1.0	3
742	The T-Cell Receptor Can Bind to the Peptide-Bound Major Histocompatibility Complex and Uncomplexed Î²₂-Microglobulin through Distinct Binding Sites. <i>Biochemistry</i> , 2017, 56, 3945-3961.	1.2	8
743	Efficient conformational sampling and weak scoring in docking programs? Strategy of the wisdom of crowds. <i>Journal of Cheminformatics</i> , 2017, 9, 37.	2.8	44
744	Multiple molecular dynamics simulations of human LOX-1 and Trp150Ala mutant reveal the structural determinants causing the full deactivation of the receptor. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1902-1912.	1.5	1
745	Membrane localization and dynamics of geranylgeranylated Rab5 hypervariable region. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 1335-1349.	1.4	18
746	Crowding in Cellular Environments at an Atomistic Level from Computer Simulations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8009-8025.	1.2	136
747	Eicosapentaenoic acid modulates the synergistic action of CREB1 and ID/E2A family members in the rat pup brain and mouse embryonic stem cells. <i>Biochimica Et Biophysica Acta - Gene Regulatory Mechanisms</i> , 2017, 1860, 870-884.	0.9	1

#	ARTICLE	IF	CITATIONS
748	Prediction of Bond Vector Autocorrelation Functions from Larmor Frequency-Selective Order Parameter Analysis of NMR Relaxation Data. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3276-3289.	2.3	13
749	Temperature dependence of protein-water interactions in a gated yeast aquaporin. <i>Scientific Reports</i> , 2017, 7, 4016.	1.6	9
750	Skeletal Dysplasia Mutations Effect on Human Filaminsâ€™™ Structure and Mechanosensing. <i>Scientific Reports</i> , 2017, 7, 4218.	1.6	13
751	Conformational Heterogeneity of the HIV Envelope Glycan Shield. <i>Scientific Reports</i> , 2017, 7, 4435.	1.6	32
752	A QM/MM study on the enzymatic inactivation of cefotaxime. <i>Journal of Molecular Modeling</i> , 2017, 23, 209.	0.8	6
753	The I427T neuraminidase (NA) substitution, located outside the NA active site of an influenza A(H1N1)pdm09 variant with reduced susceptibility to NA inhibitors, alters NA properties and impairs viral fitness. <i>Antiviral Research</i> , 2017, 137, 6-13.	1.9	11
754	Computer-Aided Drug Design Methods. <i>Methods in Molecular Biology</i> , 2017, 1520, 85-106.	0.4	317
755	In Silico Methods for Analyzing Mutagenesis Targets. <i>Methods in Molecular Biology</i> , 2017, 1498, 199-226.	0.4	1
756	Disease-causing point-mutations in metal-binding domains of Wilson disease protein decrease stability and increase structural dynamics. <i>BioMetals</i> , 2017, 30, 27-35.	1.8	13
757	Estimation of relative free energies of binding using preâ€™computed ensembles based on the singleâ€™step free energy perturbation and the siteâ€™identification by Ligand competitive saturation approaches. <i>Journal of Computational Chemistry</i> , 2017, 38, 1238-1251.	1.5	26
758	Microsecond simulation of human aquaporin 2 reveals structural determinants of water permeability and selectivity. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 10-16.	1.4	16
759	Identification of a novel lipid binding motif in apolipoprotein B by the analysis of hydrophobic cluster domains. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 135-145.	1.4	13
760	Protein Folding and Structure Prediction from the Ground Up II: AAWSEM for Î±/Î² Proteins. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3473-3482.	1.2	21
761	CHARMM36m: an improved force field for folded and intrinsically disordered proteins. <i>Nature Methods</i> , 2017, 14, 71-73.	9.0	3,959
762	Comparison of force fields for Alzheimer's A: A case study for intrinsically disordered proteins. <i>Protein Science</i> , 2017, 26, 174-185.	3.1	118
763	Error assessment in molecular dynamics trajectories using computed NMR chemical shifts. <i>Computational and Theoretical Chemistry</i> , 2017, 1099, 152-166.	1.1	1
764	Role of Acetylcholinesterase in Î²-Amyloid Aggregation Studied by Accelerated Molecular Dynamics. <i>BioNanoScience</i> , 2017, 7, 396-402.	1.5	23
765	CHARMMâ€™GUI 10 years for biomolecular modeling and simulation. <i>Journal of Computational Chemistry</i> , 2017, 38, 1114-1124.	1.5	224

#	ARTICLE	IF	CITATIONS
766	Editorâ€™s Highlight: Microbial-Derived 1,4-Dihydroxy-2-naphthoic Acid and Related Compounds as Aryl Hydrocarbon Receptor Agonists/Antagonists: Structureâ€™Activity Relationships and Receptor Modeling. <i>Toxicological Sciences</i> , 2017, 155, 458-473.	1.4	40
767	Computing infrared spectra of proteins using the exciton model. <i>Journal of Computational Chemistry</i> , 2017, 38, 1362-1375.	1.5	23
768	Conformational Preference of Serogroup B <i>Salmonella</i> O Polysaccharide in Presence and Absence of the Monoclonal Antibody Se155â€™4. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3412-3423.	1.2	11
769	Coupling between ATP hydrolysis and protein conformational change in maltose transporter. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 207-220.	1.5	0
770	Search for approaches to improving the calculation accuracy of the proteinâ€™ligand binding energy by docking. <i>Russian Chemical Bulletin</i> , 2017, 66, 1913-1924.	0.4	13
771	Active-site protein dynamics and solvent accessibility in native <i>Achromobacter cycloclastes</i> copper nitrite reductase. <i>IUCrj</i> , 2017, 4, 495-505.	1.0	11
772	Protonation Enhances the Inherent Helix-Forming Propensity of pHLIP. <i>ACS Omega</i> , 2017, 2, 8536-8542.	1.6	12
773	Conformational disorder and solvation properties of the key-residues of a protein in waterâ€™ethanol mixed solutions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32636-32646.	1.3	4
774	Atomistic Insights into Structural Differences between E3 and E4 Isoforms of Apolipoprotein E. <i>Biophysical Journal</i> , 2017, 113, 2682-2694.	0.2	17
775	Complete proteinâ€™protein association kinetics in atomic detail revealed by molecular dynamics simulations and Markov modelling. <i>Nature Chemistry</i> , 2017, 9, 1005-1011.	6.6	304
776	Hydroxyl-radical footprinting combined with molecular modeling identifies unique features of DNA conformation and nucleosome positioning. <i>Nucleic Acids Research</i> , 2017, 45, 9229-9243.	6.5	18
777	Ascorbic acid may not be involved in cryptochrome-based magnetoreception. <i>Journal of the Royal Society Interface</i> , 2017, 14, 20170657.	1.5	25
778	The complex of PAMAM-OH dendrimer with Angiotensin (1–7) prevented the disuse-induced skeletal muscle atrophy in mice. <i>International Journal of Nanomedicine</i> , 2017, Volume 12, 1985-1999.	3.3	29
779	Asymmetry of inverted-topology repeats in the AE1 anion exchanger suggests an elevator-like mechanism. <i>Journal of General Physiology</i> , 2017, 149, 1149-1164.	0.9	32
780	The First Extracellular Linker Is Important for Several Aspects of the Gating Mechanism of Human TRPA1 Channel. <i>Frontiers in Molecular Neuroscience</i> , 2017, 10, 16.	1.4	19
781	Design and Characterization of a Human Monoclonal Antibody that Modulates Mutant Connexin 26 Hemichannels Implicated in Deafness and Skin Disorders. <i>Frontiers in Molecular Neuroscience</i> , 2017, 10, 298.	1.4	31
782	His-FLAG Tag as a Fusion Partner of Glycosylated Human Interferon-Gamma and Its Mutant: Gain or Loss?. <i>BioMed Research International</i> , 2017, 2017, 1-12.	0.9	4
783	Atomistic simulations indicate the c-subunit ring of the F1Fo ATP synthase is not the mitochondrial permeability transition pore. <i>ELife</i> , 2017, 6, .	2.8	71

#	ARTICLE	IF	CITATIONS
784	The DRF motif of CXCR6 as chemokine receptor adaptation to adhesion. PLoS ONE, 2017, 12, e0173486.	1.1	23
785	The influence of cell membrane and SNAP25 linker loop on the dynamics and unzipping of SNARE complex. PLoS ONE, 2017, 12, e0176235.	1.1	8
786	Involvement of arginine 878 together with Ca ²⁺ in mouse aminopeptidase A substrate specificity for N-terminal acidic amino-acid residues. PLoS ONE, 2017, 12, e0184237.	1.1	5
787	OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. PLoS Computational Biology, 2017, 13, e1005659.	1.5	1,561
788	Water permeation through the internal water pathway in activated GPCR rhodopsin. PLoS ONE, 2017, 12, e0176876.	1.1	14
789	An evolutionary analysis identifies a conserved pentapeptide stretch containing the two essential lysine residues for rice L-myo-inositol 1-phosphate synthase catalytic activity. PLoS ONE, 2017, 12, e0185351.	1.1	22
790	Polymodal allosteric regulation of Type 1 Serine/Threonine Kinase Receptors via a conserved electrostatic lock. PLoS Computational Biology, 2017, 13, e1005711.	1.5	16
791	Recent Progress in Free Energy Methods. , 2017, , 34-50.		3
792	Transmembrane motions of PglB induced by LLO are coupled with EL5 loop conformational changes necessary for OST activity. Glycobiology, 2017, 27, 787-787.	1.3	3
793	Advances in Molecular Simulation. , 2017, , 14-33.		1
794	Biomining of MoS ₂ with Peptide-based Smart Biomaterials. Scientific Reports, 2018, 8, 3374.	1.6	23
795	Fixed-Charge Atomistic Force Fields for Molecular Dynamics Simulations in the Condensed Phase: An Overview. Journal of Chemical Information and Modeling, 2018, 58, 565-578.	2.5	144
796	Ultra-thin enzymatic liquid membrane for CO ₂ separation and capture. Nature Communications, 2018, 9, 990.	5.8	62
797	Blood Proteins and Their Interactions with Nanoparticles Investigated Using Molecular Dynamics Simulations. , 2018, , 5-19.		0
798	Permeability and ammonia selectivity in aquaporin TIP2;1: linking structure to function. Scientific Reports, 2018, 8, 2995.	1.6	24
799	New developments in force fields for biomolecular simulations. Current Opinion in Structural Biology, 2018, 49, 129-138.	2.6	181
800	Impact of Edge Groups on the Hydration and Aggregation Properties of Graphene Oxide. Journal of Physical Chemistry B, 2018, 122, 2578-2586.	1.2	15
801	Exploring the Viral Channel KcvPBCV-1 Function via Computation. Journal of Membrane Biology, 2018, 251, 419-430.	1.0	10

#	ARTICLE	IF	CITATIONS
802	On the distinct binding modes of expansin and carbohydrate-binding module proteins on crystalline and nanofibrous cellulose: implications for cellulose degradation by designer cellulosomes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8278-8293.	1.3	12
803	Computed Free Energies of Peptide Insertion into Bilayers are Independent of Computational Method. <i>Journal of Membrane Biology</i> , 2018, 251, 345-356.	1.0	22
804	New tricks for old dogs: improving the accuracy of biomolecular force fields by pair-specific corrections to non-bonded interactions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 8432-8449.	1.3	180
805	Mutational Analysis of Neuropeptide Y Reveals Unusual Thermal Stability Linked to Higher-Order Self-Association. <i>ACS Omega</i> , 2018, 3, 2141-2154.	1.6	11
806	Integrating NMR, SAXS, and Atomistic Simulations: Structure and Dynamics of a Two-Domain Protein. <i>Biophysical Journal</i> , 2018, 114, 839-855.	0.2	20
807	Deciphering complex dynamics of water counteraction around secondary structural elements of allosteric protein complex: Case study of SAP-SLAM system in signal transduction cascade. <i>Journal of Chemical Physics</i> , 2018, 148, 045102.	1.2	1
808	Transient receptor potential vanilloid 4 (TRPV4) activation by arachidonic acid requires protein kinase A-mediated phosphorylation. <i>Journal of Biological Chemistry</i> , 2018, 293, 5307-5322.	1.6	47
809	Structure refinement of membrane proteins via molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 738-750.	1.5	15
810	dbSWEET: An Integrated Resource for SWEET Superfamily to Understand, Analyze and Predict the Function of Sugar Transporters in Prokaryotes and Eukaryotes. <i>Journal of Molecular Biology</i> , 2018, 430, 2203-2211.	2.0	7
811	Antioxidant and cytotoxic activity of new di- and polyamine caffeine analogues. <i>Free Radical Research</i> , 2018, 52, 724-736.	1.5	10
812	Conditional Protein Splicing Switch in Hyperthermophiles through an Intein-Extein Partnership. <i>MBio</i> , 2018, 9, .	1.8	26
813	Accurate Methyl Group Dynamics in Protein Simulations with AMBER Force Fields. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5038-5048.	1.2	38
814	Structure of the alternative complex III in a supercomplex with cytochrome oxidase. <i>Nature</i> , 2018, 557, 123-126.	13.7	198
815	Can 2,2,2-trifluoroethanol be an efficient protein denaturant than methanol and ethanol under thermal stress?. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 9886-9896.	1.3	15
816	Folding a viral peptide in different membrane environments: pathway and sampling analyses. <i>Journal of Biological Physics</i> , 2018, 44, 195-209.	0.7	6
817	Molecular dynamics simulations of site point mutations in the TPR domain of cyclophilin 40 identify conformational states with distinct dynamic and enzymatic properties. <i>Journal of Chemical Physics</i> , 2018, 148, 145101.	1.2	12
818	A1603P and K1617del, Mutations in β^2 -Cardiac Myosin Heavy Chain that Cause Laing Early-Onset Distal Myopathy, Affect Secondary Structure and Filament Formation In Vitro and In Vivo. <i>Journal of Molecular Biology</i> , 2018, 430, 1459-1478.	2.0	12
819	Absolute Alchemical Free Energy Calculations for Ligand Binding: A Beginner's Guide. <i>Methods in Molecular Biology</i> , 2018, 1762, 199-232.	0.4	38

#	ARTICLE	IF	CITATIONS
820	A subset of functional adaptation mutations alter propensity for α -helical conformation in the intrinsically disordered glucocorticoid receptor tau1 core activation domain. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2018, 1862, 1452-1461.	1.1	8
821	Counting charges on membrane-bound peptides. <i>Chemical Science</i> , 2018, 9, 4285-4298.	3.7	23
822	Exploring conformational states and helical packings in the P2X receptor transmembrane domain by molecular dynamics simulation. <i>Journal of Biological Physics</i> , 2018, 44, 331-344.	0.7	1
823	Effect of osmolytes on the thermal stability of proteins: replica exchange simulations of Trp-cage in urea and betaine solutions. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 11174-11182.	1.3	18
824	Mutations Alter RNA-Mediated Conversion of Human Prions. <i>ACS Omega</i> , 2018, 3, 3936-3944.	1.6	6
825	Membrane plasticity facilitates recognition of the inhibitor oligomycin by the mitochondrial ATP synthase rotor. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2018, 1859, 789-796.	0.5	6
826	Micellar confinement disrupts collective structure and accelerates collective dynamics of encapsulated water. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 11454-11469.	1.3	19
827	Roles of conserved tryptophans in trimerization of HIV-1 membrane-proximal external regions: Implications for virucidal design via alchemical free-energy molecular simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 707-711.	1.5	4
828	High-resolution cryo-EM analysis of the yeast ATP synthase in a lipid membrane. <i>Science</i> , 2018, 360, .	6.0	163
829	DNP-Enhanced MAS NMR: A Tool to Snapshot Conformational Ensembles of α -Synuclein in Different States. <i>Biophysical Journal</i> , 2018, 114, 1614-1623.	0.2	38
830	Molecular Modeling of Chemoreceptor:Ligand Interactions. <i>Methods in Molecular Biology</i> , 2018, 1729, 353-372.	0.4	4
831	Comparative CHARMM and AMOEBA Simulations of Lanthanide Hydration Energetics and Experimental Aqueous-Solution Structures. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1781-1790.	2.3	28
832	Structural properties of apolipoprotein A-I mimetic peptides that promote ABCA1-dependent cholesterol efflux. <i>Scientific Reports</i> , 2018, 8, 2956.	1.6	27
833	Rapid Convergence of Energy and Free Energy Profiles with Quantum Mechanical Size in Quantum Mechanical-Molecular Mechanical Simulations of Proton Transfer in DNA. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1695-1705.	2.3	34
834	Simulating the β -secretase enzyme: Recent advances and future directions. <i>Biochimie</i> , 2018, 147, 130-135.	1.3	14
835	Prediction of the Hydrogen Peroxide-Induced Methionine Oxidation Propensity in Monoclonal Antibodies. <i>Journal of Pharmaceutical Sciences</i> , 2018, 107, 1282-1289.	1.6	25
836	Multiple Pathways and Time Scales for Conformational Transitions in apo-Adenylate Kinase. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1716-1726.	2.3	25
837	Anomalous dynamics of interfacial water around micelles. <i>Physica B: Condensed Matter</i> , 2018, 551, 167-171.	1.3	2

#	ARTICLE	IF	CITATIONS
838	Assessing AMBER force fields for protein folding in an implicit solvent. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7206-7216.	1.3	35
839	Quasiharmonic Analysis of the Energy Landscapes of Dihydrofolate Reductase from Piezophiles and Mesophiles. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5527-5533.	1.2	6
840	Selectivity and Mechanism of Fengycin, an Antimicrobial Lipopeptide, from Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2018, 122, 2219-2226.	1.2	62
841	A dual role for the N-terminal domain of the IL-3 receptor in cell signalling. <i>Nature Communications</i> , 2018, 9, 386.	5.8	28
842	Allosteric Modulation of Human Hsp90's Conformational Dynamics. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 383-404.	2.5	79
843	Structural basis of the molecular ruler mechanism of a bacterial glycosyltransferase. <i>Nature Communications</i> , 2018, 9, 445.	5.8	31
844	Predicting protein's DNA binding free energy change upon missense mutations using modified MM/PBSA approach: SAMPDI webserver. <i>Bioinformatics</i> , 2018, 34, 779-786.	1.8	55
845	Toward rational antibody design: recent advancements in molecular dynamics simulations. <i>International Immunology</i> , 2018, 30, 133-140.	1.8	39
846	Hydration Behavior along the Folding Pathways of Trpzip4, Trpzip5 and Trpzip6. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1560-1572.	1.2	6
847	Structural basis for chitin acquisition by marine <i>Vibrio</i> species. <i>Nature Communications</i> , 2018, 9, 220.	5.8	37
848	Phosphorylation induced cochaperone unfolding promotes kinase recruitment and client class-specific Hsp90 phosphorylation. <i>Nature Communications</i> , 2018, 9, 265.	5.8	39
849	Inhibition of the proteasome activity by graphene oxide contributes to its cytotoxicity. <i>Nanotoxicology</i> , 2018, 12, 185-200.	1.6	14
850	A high-throughput and rapid computational method for screening of RNA post-transcriptional modifications that can be recognized by target proteins. <i>Methods</i> , 2018, 143, 34-47.	1.9	8
851	Balancing Force Field Protein's Lipid Interactions To Capture Transmembrane Helix's Helix Association. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1706-1715.	2.3	40
852	Universal kinetic solvent effects in acid-catalyzed reactions of biomass-derived oxygenates. <i>Energy and Environmental Science</i> , 2018, 11, 617-628.	15.6	122
853	Structural Modulation of Human Amylin Protofilaments by Naturally Occurring Mutations. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5657-5665.	1.2	11
854	Molecular mechanism for inhibition of twinfilin by phosphoinositides. <i>Journal of Biological Chemistry</i> , 2018, 293, 4818-4829.	1.6	15
855	Revisiting the earliest signatures of amyloidogenesis: Roadmaps emerging from computational modeling and experiment. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1359.	6.2	17

#	ARTICLE	IF	CITATIONS
856	Structural Impact of Phosphorylation and Dielectric Constant Variation on Synaptotagmin's IDR. <i>Biophysical Journal</i> , 2018, 114, 550-561.	0.2	13
857	Molecular details of spontaneous insertion and interaction of HCV non-structure 3 protease protein domain with PIP2-containing membrane. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 423-433.	1.5	1
858	Development of CHARMM-Compatible Force-Field Parameters for Cobalamin and Related Cofactors from Quantum Mechanical Calculations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 784-798.	2.3	20
859	The action of a negative allosteric modulator at the dopamine D2 receptor is dependent upon sodium ions. <i>Scientific Reports</i> , 2018, 8, 1208.	1.6	16
860	Structural flexibility and protein adaptation to temperature: Molecular dynamics analysis of malate dehydrogenases of marine molluscs. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 1274-1279.	3.3	204
861	The structural determinants of the bitopic binding mode of a negative allosteric modulator of the dopamine D 2 receptor. <i>Biochemical Pharmacology</i> , 2018, 148, 315-328.	2.0	26
862	Double-Cone Localization and Seasonal Expression Pattern Suggest a Role in Magnetoreception for European Robin Cryptochrome 4. <i>Current Biology</i> , 2018, 28, 211-223.e4.	1.8	134
863	Structural basis of TRPV5 channel inhibition by econazole revealed by cryo-EM. <i>Nature Structural and Molecular Biology</i> , 2018, 25, 53-60.	3.6	114
864	G4941K substitution in the pore-lining S6 helix of the skeletal muscle ryanodine receptor increases RyR1 sensitivity to cytosolic and luminal Ca ²⁺ . <i>Journal of Biological Chemistry</i> , 2018, 293, 2015-2028.	1.6	10
865	Estimation of structure and stability of MurE ligase from <i>Salmonella enterica</i> serovar Typhi. <i>International Journal of Biological Macromolecules</i> , 2018, 109, 375-382.	3.6	5
866	Solution structure of an ultra-stable single-chain insulin analog connects protein dynamics to a novel mechanism of receptor binding. <i>Journal of Biological Chemistry</i> , 2018, 293, 69-88.	1.6	12
867	Multifunnel Landscape of the Fold-Switching Protein RfaH-CTD. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1600-1607.	1.2	26
868	Advantages of a distant cellulase catalytic base. <i>Journal of Biological Chemistry</i> , 2018, 293, 4680-4687.	1.6	5
869	Phosphorylation-mediated structural changes within the SOAR domain of stromal interaction molecule 1 enable specific activation of distinct Orai channels. <i>Journal of Biological Chemistry</i> , 2018, 293, 3145-3155.	1.6	11
870	Binding Specificity Determines the Cytochrome P450 3A4 Mediated Enantioselective Metabolism of Metconazole. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1176-1184.	1.2	29
871	High-strength, Durable All-Silk Fibroin Hydrogels with Versatile Processability toward Multifunctional Applications. <i>Advanced Functional Materials</i> , 2018, 28, 1704757.	7.8	133
872	Mechanism and Determinants of Amphipathic Helix-Containing Protein Targeting to Lipid Droplets. <i>Developmental Cell</i> , 2018, 44, 73-86.e4.	3.1	175
873	Identification of Factors Promoting HBV Capsid Self-Assembly by Assembly-Promoting Antivirals. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 328-337.	2.5	12

#	ARTICLE	IF	CITATIONS
874	pH-Dependent cooperativity and existence of a dry molten globule in the folding of a miniprotein BBL. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3523-3530.	1.3	10
875	BIM Binding Remotely Regulates BAX Activation: Insights from the Free Energy Landscapes. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 370-382.	2.5	5
876	The protease GtgE from <i>Salmonella</i> exclusively targets inactive Rab GTPases. <i>Nature Communications</i> , 2018, 9, 44.	5.8	33
877	Structure of the Nanobody-Stabilized Active State of the Kappa Opioid Receptor. <i>Cell</i> , 2018, 172, 55-67.e15.	13.5	299
878	Unbiased Molecular Dynamics of 11 min Timescale Drug Unbinding Reveals Transition State Stabilizing Interactions. <i>Journal of the American Chemical Society</i> , 2018, 140, 618-628.	6.6	107
879	Enhanced configurational sampling with hybrid non-equilibrium molecular dynamicsâ€œMonte Carlo propagator. <i>Journal of Chemical Physics</i> , 2018, 148, 014101.	1.2	26
880	Theoretical insights on the inhibition mechanism of a class A Serine Hydrolase by avibactam. <i>Journal of Computational Chemistry</i> , 2018, 39, 1943-1948.	1.5	6
881	Molecular dynamics simulations of lipid nanodiscs. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 2094-2107.	1.4	24
882	Refining Markov state models for conformational dynamics using ensemble-averaged data and time-series trajectories. <i>Journal of Chemical Physics</i> , 2018, 148, 241731.	1.2	11
883	Molecular mechanism of GPCR-mediated arrestin activation. <i>Nature</i> , 2018, 557, 452-456.	13.7	166
884	Phosphatidylinositol-3,5-bisphosphate lipid-binding-induced activation of the human two-pore channel 2. <i>Cellular and Molecular Life Sciences</i> , 2018, 75, 3803-3815.	2.4	28
885	Critical Role of the Human T-Cell Leukemia Virus Type 1 Capsid N-Terminal Domain for Gag-Gag Interactions and Virus Particle Assembly. <i>Journal of Virology</i> , 2018, 92, .	1.5	10
886	Computer-Aided Drug Discovery. , 2018, , 7-24.		11
887	Protein Partitioning into Ordered Membrane Domains: Insights from Simulations. <i>Biophysical Journal</i> , 2018, 114, 1936-1944.	0.2	63
888	Enhanced Monte Carlo Methods for Modeling Proteins Including Computation of Absolute Free Energies of Binding. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3279-3288.	2.3	35
889	Tertiary structure of apolipoprotein A-I in nascent high-density lipoproteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 5163-5168.	3.3	35
890	Control of Integrin Affinity by Confining RGD Peptides on Fluorescent Carbon Nanotubes. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 17693-17703.	4.0	47
892	Molecular mechanism of extreme mechanostability in a pathogen adhesin. <i>Science</i> , 2018, 359, 1527-1533.	6.0	176

#	ARTICLE	IF	CITATIONS
893	A trapped human PPM1A phosphopeptide complex reveals structural features critical for regulation of PPM protein phosphatase activity. <i>Journal of Biological Chemistry</i> , 2018, 293, 7993-8008.	1.6	19
894	Cations Modulate Actin Bundle Mechanics, Assembly Dynamics, and Structure. <i>Journal of Physical Chemistry B</i> , 2018, 122, 3826-3835.	1.2	21
895	On the Calculation of SAXS Profiles of Folded and Intrinsically Disordered Proteins from Computer Simulations. <i>Journal of Molecular Biology</i> , 2018, 430, 2521-2539.	2.0	64
896	Transferable Neural Networks for Enhanced Sampling of Protein Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1887-1894.	2.3	77
897	NAMD goes quantum: an integrative suite for hybrid simulations. <i>Nature Methods</i> , 2018, 15, 351-354.	9.0	149
898	Catalytic mechanism and molecular engineering of quinolone biosynthesis in dioxygenase AsqJ. <i>Nature Communications</i> , 2018, 9, 1168.	5.8	30
899	Molecular Mechanics Parameterization of Anesthetic Molecules. <i>Methods in Enzymology</i> , 2018, 602, 61-76.	0.4	3
900	Aggregation of PrP106 ¹²⁶ on surfaces of neutral and negatively charged membranes studied by molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 1936-1948.	1.4	5
901	A local instantaneous surface method for extracting membrane elastic moduli from simulation: Comparison with other strategies. <i>Chemical Physics</i> , 2018, 514, 31-43.	0.9	22
902	A new method for finding the minimum free energy pathway of ions and small molecule transportation through protein based on 3D-RISM theory and the string method. <i>Chemical Physics Letters</i> , 2018, 699, 22-27.	1.2	4
903	Escape of a Small Molecule from Inside T4 Lysozyme by Multiple Pathways. <i>Biophysical Journal</i> , 2018, 114, 1058-1066.	0.2	44
904	Elucidating the multi-targeted anti-amyloid activity and enhanced islet amyloid polypeptide binding of Î²-wrapins. <i>Computers and Chemical Engineering</i> , 2018, 116, 322-332.	2.0	13
905	Modeling Protein Aromatic Motifs Reveals Their Structural and Redox Flexibility. <i>Journal of Physical Chemistry B</i> , 2018, 122, 3760-3770.	1.2	22
906	Elucidating the amphiphilic character of graphene oxide. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 9507-9515.	1.3	40
907	Predicting rates of <i>in vivo</i> degradation of recombinant spider silk proteins. <i>Journal of Tissue Engineering and Regenerative Medicine</i> , 2018, 12, e97-e105.	1.3	21
908	Molecular dynamics analysis of the structural and dynamic properties of the functionally enhanced hepta-variant of mouse 5-aminolevulinic synthase. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 152-165.	2.0	4
909	Optically sensing phospholipid induced coil-helix transitions in the phosphoinositide-binding motif of gelsolin. <i>Faraday Discussions</i> , 2018, 207, 437-458.	1.6	5
910	Optical backbone-sidechain charge transfer transitions in proteins sensitive to secondary structure and modifications. <i>Faraday Discussions</i> , 2018, 207, 115-135.	1.6	17

#	ARTICLE	IF	CITATIONS
911	Assessment of the model refinement category in CASP12. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 152-167.	1.5	33
912	Finding the needle in the haystack: towards solving the protein-folding problem computationally. <i>Critical Reviews in Biochemistry and Molecular Biology</i> , 2018, 53, 1-28.	2.3	31
913	CDOCKER and λ -dynamics for prospective prediction in D3R Grand Challenge 2. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 89-102.	1.3	9
914	Hinge action versus grip in translocation by RNA polymerase. <i>Transcription</i> , 2018, 9, 1-16.	1.7	10
915	Importance of the second extracellular loop for melatonin MT ₁ receptor function and absence of melatonin binding in GPR50. <i>British Journal of Pharmacology</i> , 2018, 175, 3281-3297.	2.7	23
916	Calculation of conformational free energies by confinement simulations in explicit water with implicit desolvation. <i>Molecular Simulation</i> , 2018, 44, 1082-1089.	0.9	3
917	The role of caveolin-1 in lipid droplets and their biogenesis. <i>Chemistry and Physics of Lipids</i> , 2018, 211, 93-99.	1.5	18
918	Conformational dynamics and free energy of BHRF1 binding to Bim BH3. <i>Biophysical Chemistry</i> , 2018, 232, 22-28.	1.5	6
919	Simulations of simple Bovine and Homo sapiens outer cortex ocular lens membrane models with a majority concentration of cholesterol. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 2134-2144.	1.4	16
920	Structure-inspired design of β^2 -arrestin-biased ligands for aminergic GPCRs. <i>Nature Chemical Biology</i> , 2018, 14, 126-134.	3.9	141
921	Effects of force fields on the conformational and dynamic properties of amyloid β (1-40) dimer explored by replica exchange molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 279-300.	1.5	23
922	Thermodynamics of Amyloid- β Fibril Elongation: Atomistic Details of the Transition State. <i>ACS Chemical Neuroscience</i> , 2018, 9, 783-789.	1.7	33
923	Concentration-dependent binding of CdSe quantum dots on the SH3 domain. <i>Nanoscale</i> , 2018, 10, 351-358.	2.8	8
924	Novel 2-(2-arylmethylthio-4-chloro-5-methylbenzenesulfonyl)-1-(1,3,5-triazin-2-ylamino)guanidine derivatives: Inhibition of human carbonic anhydrase cytosolic isozymes I and II and the transmembrane tumor-associated isozymes IX and XII, anticancer activity, and molecular modeling studies. <i>European Journal of Medicinal Chemistry</i> , 2018, 143, 1931-1941.	2.6	26
925	Force field development and simulations of intrinsically disordered proteins. <i>Current Opinion in Structural Biology</i> , 2018, 48, 40-48.	2.6	139
926	Protein structure-based drug design: from docking to molecular dynamics. <i>Current Opinion in Structural Biology</i> , 2018, 48, 93-102.	2.6	405
927	Computer-aided design of human sialyltransferase inhibitors of hST8Sia III. <i>Journal of Molecular Recognition</i> , 2018, 31, e2684.	1.1	8
928	Molecular dynamics simulation of the thermosensitivity of the human connexin 26 hemichannel. <i>Chemical Physics</i> , 2018, 500, 7-14.	0.9	7

#	ARTICLE	IF	CITATIONS
929	A QM/MM Study of Nitrite Binding Modes in a Three-Domain Heme-Cu Nitrite Reductase. <i>Molecules</i> , 2018, 23, 2997.	1.7	5
930	Role of protein interactions in stabilizing canonical DNA features in simulations of DNA in crowded environments. <i>BMC Biophysics</i> , 2018, 11, 8.	4.4	7
931	Molecular dynamics simulation of the follicle-stimulating hormone receptor. Understanding the conformational dynamics of receptor variants at positions N680 and D408 from in silico analysis. <i>PLoS ONE</i> , 2018, 13, e0207526.	1.1	8
932	Computational biochemical investigation of the binding energy interactions between an estrogen receptor and its agonists. <i>New Journal of Chemistry</i> , 2018, 42, 19801-19810.	1.4	10
933	Probing the binding mode and unbinding mechanism of LSD1 inhibitors by combined computational methods. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 29833-29846.	1.3	1
934	Influence of membrane lipid composition on the structure and activity of I^3 -secretase. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27294-27304.	1.3	20
935	Theoretical rationalisation of the photophysics of a TICT excited state of cinnamoyl coumarin derivatives in homogeneous and biological membrane models. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27621-27629.	1.3	10
936	Precise estimation of transfer free energies for ionic species between similar media. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27003-27010.	1.3	1
937	Quantifying the influence of the ion cloud on SAXS profiles of charged proteins. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26351-26361.	1.3	9
938	Molecular simulations reveal that a short helical loop regulates thermal stability of type I cohesin-dockerin complexes. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28445-28451.	1.3	3
939	Protein structure networks provide insight into active site flexibility in esterase/lipases from the carnivorous plant <i>Drosera capensis</i> . <i>Integrative Biology (United Kingdom)</i> , 2018, 10, 768-779.	0.6	10
940	Protein Design Assisted Residue Conservation and Functional Stability Analysis for Bacterial Chemotaxis. , 2018, , .		0
941	Dynamic recognition and linkage specificity in K63 di-ubiquitin and TAB2 NZF domain complex. <i>Scientific Reports</i> , 2018, 8, 16478.	1.6	3
942	Exploring Peptide-Solvent Interactions: A Computational Study. <i>Molecules</i> , 2018, 23, 2355.	1.7	1
943	Representation of the QM Subsystem for Long-Range Electrostatic Interaction in Non-Periodic Ab Initio QM/MM Calculations. <i>Molecules</i> , 2018, 23, 2500.	1.7	8
944	Conservation of Potentially Druggable Cavities in Intrinsically Disordered Proteins. <i>ACS Omega</i> , 2018, 3, 15643-15652.	1.6	22
945	Identification of molecular determinants that govern distinct STIM2 activation dynamics. <i>PLoS Biology</i> , 2018, 16, e2006898.	2.6	29
946	Dual Role of the C-Terminal Domain in Osmosensing by Bacterial Osmolyte Transporter ProP. <i>Biophysical Journal</i> , 2018, 115, 2152-2166.	0.2	11

#	ARTICLE	IF	CITATIONS
947	Heavy Anionic Complex Creates a Unique Water Structure at a Soft Charged Interface. <i>Journal of Physical Chemistry C</i> , 2018, 122, 29228-29236.	1.5	29
948	Atomistic Peptide Folding Simulations Reveal Interplay of Entropy and Long-Range Interactions in Folding Cooperativity. <i>Scientific Reports</i> , 2018, 8, 13668.	1.6	7
949	Molecular Mechanism for the Role of the H2A and H2B Histone Tails in Nucleosome Repositioning. <i>Journal of Physical Chemistry B</i> , 2018, 122, 11827-11840.	1.2	22
950	Exploring the Ligand Efficacy of Cannabinoid Receptor 1 (CB1) using Molecular Dynamics Simulations. <i>Scientific Reports</i> , 2018, 8, 13787.	1.6	25
951	Calcium interactions with Cx26 hemmichannel: Spatial association between MD simulations biding sites and variant pathogenicity. <i>Computational Biology and Chemistry</i> , 2018, 77, 331-342.	1.1	9
952	On the Mechanism of Action of Anti-Inflammatory Activity of Hypericin: An In Silico Study Pointing to the Relevance of Janus Kinases Inhibition. <i>Molecules</i> , 2018, 23, 3058.	1.7	20
953	Calcium stabilizes the strongest protein fold. <i>Nature Communications</i> , 2018, 9, 4764.	5.8	41
954	Three Weaknesses for Three Perturbations: Comparing Protein Unfolding Under Shear, Force, and Thermal Stresses. <i>Journal of Physical Chemistry B</i> , 2018, 122, 11922-11930.	1.2	24
955	Structural Basis for the Limited Response to Oxidative and Thiol-Conjugating Agents by Triosephosphate Isomerase From the Photosynthetic Bacteria <i>Synechocystis</i> . <i>Frontiers in Molecular Biosciences</i> , 2018, 5, 103.	1.6	5
956	Molecular dynamics simulations of nucleotide release from the circadian clock protein KaiC reveal atomic-resolution functional insights. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E11475-E11484.	3.3	24
957	Evolutionary Effects on Bound Substrate p <i>K</i> _a in Dihydrofolate Reductase. <i>Journal of the American Chemical Society</i> , 2018, 140, 16650-16660.	6.6	17
958	Single Molecular Layer of Silk Nanoribbon as Potential Basic Building Block of Silk Materials. <i>ACS Nano</i> , 2018, 12, 11860-11870.	7.3	79
959	Simulation of Spectra of Red Fluorescent Protein Mutants. <i>Moscow University Chemistry Bulletin</i> , 2018, 73, 212-215.	0.2	4
960	Cooperative Nonbonded Forces Control Membrane Binding of the pH-Low Insertion Peptide pHLIP. <i>Biophysical Journal</i> , 2018, 115, 2403-2412.	0.2	14
961	A mutational and molecular dynamics study of the cys-loop GABA receptor Hco-UNC-49 from <i>Haemonchus contortus</i> : Agonist recognition in the nematode GABA receptor family. <i>International Journal for Parasitology: Drugs and Drug Resistance</i> , 2018, 8, 534-539.	1.4	4
962	An efficient strategy to estimate thermodynamics and kinetics of G protein-coupled receptor activation using metadynamics and maximum caliber. <i>Journal of Chemical Physics</i> , 2018, 149, 224101.	1.2	31
963	Higher Accuracy Achieved in the Simulations of Protein Structure Refinement, Protein Folding, and Intrinsically Disordered Proteins Using Polarizable Force Fields. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 7110-7116.	2.1	24
964	Transmembrane but not soluble helices fold inside the ribosome tunnel. <i>Nature Communications</i> , 2018, 9, 5246.	5.8	36

#	ARTICLE	IF	CITATIONS
965	Conformational sampling of CpxA: Connecting HAMP motions to the histidine kinase function. PLoS ONE, 2018, 13, e0207899.	1.1	1
966	Disorder in Proteins. , 2018, , .		0
967	Experimental accuracy in protein structure refinement via molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 13276-13281.	3.3	68
968	Structure of native lens connexin 46/50 intercellular channels by cryo-EM. Nature, 2018, 564, 372-377.	13.7	107
969	Propensity for Proton Relay and Electrostatic Impact of Protein Reorganization in Slr1694 BLUF Photoreceptor. Journal of the American Chemical Society, 2018, 140, 15241-15251.	6.6	25
970	Dynamic multiple-scattering treatment of X-ray absorption: Parameterization of a new molecular dynamics force field for myoglobin. Structural Dynamics, 2018, 5, 054101.	0.9	5
971	Mechanistic basis for the evolution of chalcone synthase catalytic cysteine reactivity in land plants. Journal of Biological Chemistry, 2018, 293, 18601-18612.	1.6	38
972	Hydrolysis and Transglycosylation Transition States of Glycoside Hydrolase Family 3 β -Glucosidases Differ in Charge and Puckering Conformation. Journal of Physical Chemistry B, 2018, 122, 9452-9459.	1.2	14
973	Structural evidence for the roles of divalent cations in actin polymerization and activation of ATP hydrolysis. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10345-10350.	3.3	21
974	Modeling and Mutational Analysis of the Binding Mode for the Multimodal Antidepressant Drug Vortioxetine to the Human 5-HT _{3A} Receptor. Molecular Pharmacology, 2018, 94, 1421-1434.	1.0	14
975	Systematic Comparison of Amber and Rosetta Energy Functions for Protein Structure Evaluation. Journal of Chemical Theory and Computation, 2018, 14, 6015-6025.	2.3	20
976	Peptide and Protein Structure Prediction with a Simplified Continuum Solvent Model. Journal of Physical Chemistry B, 2018, 122, 11355-11362.	1.2	1
977	Template-Guided Protein Structure Prediction and Refinement Using Optimized Folding Landscape Force Fields. Journal of Chemical Theory and Computation, 2018, 14, 6102-6116.	2.3	15
978	Heterogeneous Solvation in Distinctive Protein-Protein Interfaces Revealed by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 11695-11701.	1.2	7
979	Structure-guided design of pyridoclox derivatives based on Noxa / Mcl-1 interaction mode. European Journal of Medicinal Chemistry, 2018, 159, 357-380.	2.6	12
980	Outward open conformation of a Major Facilitator Superfamily multidrug/H ⁺ antiporter provides insights into switching mechanism. Nature Communications, 2018, 9, 4005.	5.8	46
981	Structural basis for β 1 receptor ligand recognition. Nature Structural and Molecular Biology, 2018, 25, 981-987.	3.6	109
982	A Computational Modeling Approach Predicts Interaction of the Antifungal Protein AFP from <i>Aspergillus giganteus</i> with Fungal Membranes via Its β -Core Motif. MSphere, 2018, 3, .	1.3	22

#	ARTICLE	IF	CITATIONS
983	DelPhiPKa: Including salt in the calculations and enabling polar residues to titrate. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 1277-1283.	1.5	50
984	Insights into molecular mechanisms of drug metabolism dysfunction of human CYP2C9*30. <i>PLoS ONE</i> , 2018, 13, e0197249.	1.1	24
985	Stability and Structural Analysis of A ₆ R Polypeptide Nanosheets: A Theoretical Study Using the Classical Molecular Dynamics Simulation. <i>Journal of Physical Chemistry C</i> , 2018, 122, 24445-24453.	1.5	18
986	Interactions between Triterpenes and a P-I Type Snake Venom Metalloproteinase: Molecular Simulations and Experiments. <i>Toxins</i> , 2018, 10, 397.	1.5	5
987	Design, Synthesis, Molecular Dynamics Simulation, and Functional Evaluation of a Novel Series of 26RFa Peptide Analogues Containing a Mono- or Polyalkyl Guanidino Arginine Derivative. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 10185-10197.	2.9	5
988	Probing Translocation in Mutants of the Anthrax Channel: Atomically Detailed Simulations with Milestoning. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10296-10305.	1.2	6
989	Structural and dynamic basis of substrate permissiveness in hydroxycinnamoyltransferase (HCT). <i>PLoS Computational Biology</i> , 2018, 14, e1006511.	1.5	25
990	Engineering Salt Bridge Networks between Transmembrane Helices Confers Thermostability in G-Protein-Coupled Receptors. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6574-6585.	2.3	10
991	A New Calmodulin-Binding Protein Expresses in the Context of Secondary Cell Wall Biosynthesis and Impacts Biomass Properties in <i>Populus</i> . <i>Frontiers in Plant Science</i> , 2018, 9, 1669.	1.7	31
992	Effect of Core Morphology on the Structural Asymmetry of Alkanethiol Monolayer-Protected Gold Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2018, 122, 26288-26297.	1.5	22
993	Proton Countertransport and Coupled Gating in the Sarcoplasmic Reticulum Calcium Pump. <i>Journal of Molecular Biology</i> , 2018, 430, 5050-5065.	2.0	15
994	Helical Polyampholyte Sequences Have Unique Thermodynamic Properties. <i>Journal of Physical Chemistry B</i> , 2018, 122, 11784-11791.	1.2	11
995	Storing Energy in Biodegradable Electrochemical Supercapacitors. <i>ACS Omega</i> , 2018, 3, 13869-13875.	1.6	46
996	Characterization of TDP-43 RRM2 Partially Folded States and Their Significance to ALS Pathogenesis. <i>Biophysical Journal</i> , 2018, 115, 1673-1680.	0.2	21
997	Artificial Metalloenzymes as Catalysts for Oxidative Lignin Degradation. <i>ACS Sustainable Chemistry and Engineering</i> , 2018, 6, 15100-15107.	3.2	21
998	Methionine 170 is an Environmentally Sensitive Membrane Anchor in the Disordered HVR of K-Ras4B. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10086-10096.	1.2	22
999	Molecular Characterization of Binding Loop E in the Nematode Cys-Loop GABA Receptor. <i>Molecular Pharmacology</i> , 2018, 94, 1289-1297.	1.0	6
1000	Computational Studies of Intrinsically Disordered Proteins. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10455-10469.	1.2	24

#	ARTICLE	IF	CITATIONS
1001	Asymmetric protein design from conserved supersecondary structures. <i>Journal of Structural Biology</i> , 2018, 204, 380-387.	1.3	13
1002	Molecular Dynamics Simulations of Ion Selectivity in a Claudin-15 Paracellular Channel. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10783-10792.	1.2	41
1003	Contrasting Effects of Guanidinium Chloride and Urea on the Activity and Unfolding of Lysozyme. <i>ACS Omega</i> , 2018, 3, 14119-14126.	1.6	33
1004	Direct cysteine sulfenylation drives activation of the Src kinase. <i>Nature Communications</i> , 2018, 9, 4522.	5.8	87
1005	Conformational transitions of the serotonin 5-HT ₃ receptor. <i>Nature</i> , 2018, 563, 275-279.	13.7	128
1006	Structural interpretation of DNA-protein hydroxyl-radical footprinting experiments with high resolution using HYDROID. <i>Nature Protocols</i> , 2018, 13, 2535-2556.	5.5	6
1007	Specificity landscapes unmask submaximal binding site preferences of transcription factors. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E10586-E10595.	3.3	16
1008	Inhibition of a Snake Venom Metalloproteinase by the Flavonoid Myricetin. <i>Molecules</i> , 2018, 23, 2662.	1.7	26
1009	Structural and mechanistic basis for preferential deadenylation of U6 snRNA by Usb1. <i>Nucleic Acids Research</i> , 2018, 46, 11488-11501.	6.5	16
1010	The Dimer-of-Trimers Assembly Prevents Catalysis at the Transferase Site of Prokaryotic FAD Synthase. <i>Biophysical Journal</i> , 2018, 115, 988-995.	0.2	11
1011	Optimal Hydrophobicity and Reorientation of Amphiphilic Peptides Translocating through Membrane. <i>Biophysical Journal</i> , 2018, 115, 1045-1054.	0.2	29
1012	Molecular mechanism of phosphoinositides' specificity for the inwardly rectifying potassium channel Kir2.2. <i>Chemical Science</i> , 2018, 9, 8352-8362.	3.7	2
1013	Structural elements required for coupling ion and substrate transport in the neurotransmitter transporter homolog LeuT. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E8854-E8862.	3.3	28
1014	Molecular dynamics simulations disclose early stages of the photo-activation of cryptochrome 4. <i>New Journal of Physics</i> , 2018, 20, 083018.	1.2	24
1015	Effect of late endosomal DOBMP lipid and traditional model lipids of electrophysiology on the anthrax toxin channel activity. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 2192-2203.	1.4	4
1016	Kirkwood's Buff-Derived Alcohol Parameters for Aqueous Carbohydrates and Their Application to Preferential Interaction Coefficient Calculations of Proteins. <i>Journal of Physical Chemistry B</i> , 2018, 122, 9350-9360.	1.2	17
1017	Molecular Insights into Human Hereditary Apolipoprotein A-I Amyloidosis Caused by the Glu34Lys Mutation. <i>Biochemistry</i> , 2018, 57, 5738-5747.	1.2	9
1018	Specific Residue Interactions Regulate the Binding of Dengue Antigens to Broadly Neutralizing EDE Antibodies. <i>ChemistryOpen</i> , 2018, 7, 604-610.	0.9	1

#	ARTICLE	IF	CITATIONS
1019	Insights into the role of electrostatics in temperature adaptation: a comparative study of psychrophilic, mesophilic, and thermophilic subtilisin-like serine proteases. <i>RSC Advances</i> , 2018, 8, 29698-29713.	1.7	20
1020	Mechanisms Underlying the Dual Effect of Polyunsaturated Fatty Acid Analogs on Kv7.1. <i>Cell Reports</i> , 2018, 24, 2908-2918.	2.9	39
1021	Selective Permeability of Carboxysome Shell Pores to Anionic Molecules. <i>Journal of Physical Chemistry B</i> , 2018, 122, 9110-9118.	1.2	54
1022	Assigning crystallographic electron densities with free energy calculationsâ€”The case of the fluoride channel Fluc. <i>PLoS ONE</i> , 2018, 13, e0196751.	1.1	5
1023	Phase Behavior of GM1-Containing DMPCâ€”Cholesterol Monolayer: Experimental and Theoretical Study. <i>Langmuir</i> , 2018, 34, 11602-11611.	1.6	3
1024	Engineering Ionophore Gramicidinâ€”Inspired Selfâ€”Assembled Peptides for Drug Delivery and Cancer Nanotherapeutics. <i>Advanced Therapeutics</i> , 2018, 1, 1800018.	1.6	8
1025	Approaching protein design with multisite $\langle i \rangle \hat{\lambda} \langle /i \rangle$ dynamics: Accurate and scalable mutational folding free energies in T4 lysozyme. <i>Protein Science</i> , 2018, 27, 1910-1922.	3.1	26
1026	Structural mechanisms of selectivity and gating in anion channelrhodopsins. <i>Nature</i> , 2018, 561, 349-354.	13.7	67
1027	Review of force fields and intermolecular potentials used in atomistic computational materials research. <i>Applied Physics Reviews</i> , 2018, 5, 031104.	5.5	101
1028	Structure of voltage-dependent anion channel-tethered bilayer lipid membranes determined using neutron reflectivity. <i>Acta Crystallographica Section D: Structural Biology</i> , 2018, 74, 1219-1232.	1.1	9
1029	Cloning of cDNA sequences encoding cowpea (<i>Vigna unguiculata</i>) vicilins: Computational simulations suggest a binding mode of cowpea vicilins to chitin oligomers. <i>International Journal of Biological Macromolecules</i> , 2018, 117, 565-573.	3.6	12
1030	Proline and Water Stabilization of a Universal Two-Step Folding Mechanism for $\hat{\lambda}^2$ -Turn Formation in Solution. <i>Journal of the American Chemical Society</i> , 2018, 140, 7301-7312.	6.6	9
1031	Structural basis for gating pore current in periodic paralysis. <i>Nature</i> , 2018, 557, 590-594.	13.7	55
1032	Structure and Function of the Transmembrane Domain of NsaS, an Antibiotic Sensing Histidine Kinase in <i>Staphylococcus aureus</i> . <i>Journal of the American Chemical Society</i> , 2018, 140, 7471-7485.	6.6	17
1033	QM/MM calculations reveal a bridging hydroxo group in a vanadium nitrogenase crystal structure. <i>Chemical Communications</i> , 2018, 54, 7310-7313.	2.2	51
1034	Water structure changes in oxime-mediated reactivation process of phosphorylated human acetylcholinesterase. <i>Bioscience Reports</i> , 2018, 38, .	1.1	6
1035	How accurately do force fields represent protein side chain ensembles?. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 935-944.	1.5	13
1036	Improved Force Fields for Peptide Nucleic Acids with Optimized Backbone Torsion Parameters. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3603-3620.	2.3	16

#	ARTICLE	IF	CITATIONS
1037	Intrinsically disordered protein-specific force field <sc>CHARMM</sc>36<sc>IDPSFF</sc>. Chemical Biology and Drug Design, 2018, 92, 1722-1735.	1.5	62
1038	Exploring Substrate Binding in the Extracellular Vestibule of MhsT by Atomistic Simulations and Markov Models. Journal of Chemical Information and Modeling, 2018, 58, 1244-1252.	2.5	4
1039	Unraveling the Differential Aggregation of Anionic and Nonionic Monorhamnolipids at Air-Water and Oil-Water Interfaces: A Classical Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2018, 122, 6403-6416.	1.2	21
1040	The architecture of the OmpC-MlaA complex sheds light on the maintenance of outer membrane lipid asymmetry in Escherichia coli. Journal of Biological Chemistry, 2018, 293, 11325-11340.	1.6	64
1041	Structural basis of actin monomer re-charging by cyclase-associated protein. Nature Communications, 2018, 9, 1892.	5.8	60
1042	Structure-Guided Modification of Heterocyclic Antagonists of the P2Y ₁₄ Receptor. Journal of Medicinal Chemistry, 2018, 61, 4860-4882.	2.9	32
1043	Convergent evolution of tertiary structure in rhodopsin visual proteins from vertebrates and box jellyfish. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6201-6206.	3.3	19
1044	Two distinct DNA sequences recognized by transcription factors represent enthalpy and entropy optima. ELife, 2018, 7, .	2.8	32
1045	The Solution Structure of CCL28 Reveals Structural Lability that Does Not Constrain Antifungal Activity. Journal of Molecular Biology, 2018, 430, 3266-3282.	2.0	14
1046	Structural basis for relief of phospholamban-mediated inhibition of the sarcoplasmic reticulum Ca ²⁺ -ATPase at saturating Ca ²⁺ conditions. Journal of Biological Chemistry, 2018, 293, 12405-12414.	1.6	20
1047	Energetics and conformational pathways of functional rotation in the multidrug transporter AcrB. ELife, 2018, 7, .	2.8	32
1048	A dynamic mechanism for allosteric activation of Aurora kinase A by activation loop phosphorylation. ELife, 2018, 7, .	2.8	62
1049	Assessment of ab initio models of protein complexes by molecular dynamics. PLoS Computational Biology, 2018, 14, e1006182.	1.5	33
1050	Free Energy Landscape for the Entire Transport Cycle of Triose-Phosphate/Phosphate Translocator. Structure, 2018, 26, 1284-1296.e4.	1.6	17
1051	Nanoscale Dynamics and Energetics of Proteins and Protein-Nucleic Acid Complexes in Classical Molecular Dynamics Simulations. Methods in Molecular Biology, 2018, 1814, 579-592.	0.4	0
1052	Disorder at the Tips of a Disease-Relevant A β 242 Amyloid Fibril: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2018, 122, 11072-11082.	1.2	24
1053	Force-activated catalytic pathway accelerates bacterial adhesion against flow. Biochemical Journal, 2018, 475, 2611-2620.	1.7	1
1054	Disordered peptide chains in an $\hat{\pm}$ -C-based coarse-grained model. Physical Chemistry Chemical Physics, 2018, 20, 19057-19070.	1.3	23

#	ARTICLE	IF	CITATIONS
1055	Virtual Screening of Chemical Compounds for Discovery of Complement C3 Ligands. ACS Omega, 2018, 3, 6427-6438.	1.6	15
1056	Molecular recognition of RAS/RAF complex at the membrane: Role of RAF cysteine-rich domain. Scientific Reports, 2018, 8, 8461.	1.6	71
1057	Computational simulations determining disulfonic stilbene derivative bioavailability within human serum albumin. Physical Chemistry Chemical Physics, 2018, 20, 18020-18030.	1.3	2
1058	Binding Affinity via Docking: Fact and Fiction. Molecules, 2018, 23, 1899.	1.7	292
1059	Inositol phosphates are assembly co-factors for HIV-1. Nature, 2018, 560, 509-512.	13.7	186
1060	Molecular Dynamics Simulations to Study Drug Delivery Systems. , 0, , .		10
1061	Rapid constriction of the selectivity filter underlies C-type inactivation in the KcsA potassium channel. Journal of General Physiology, 2018, 150, 1408-1420.	0.9	64
1062	C-terminal kink formation is required for lateral gating in Bama. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7942-E7949.	3.3	42
1063	Reconstitution and substrate specificity for isopentenyl pyrophosphate of the antiviral radical SAM enzyme viperin. Journal of Biological Chemistry, 2018, 293, 14122-14133.	1.6	14
1064	Alterations at Arg ⁷⁶ of human connexin 46, a residue associated with cataract formation, cause loss of gap junction formation but preserve hemichannel function. American Journal of Physiology - Cell Physiology, 2018, 315, C623-C635.	2.1	5
1065	A spin-1 representation for dual-funnel energy landscapes. Journal of Chemical Physics, 2018, 149, 035101.	1.2	2
1066	The hydration structure of methylthiolate from QM/MM molecular dynamics. Journal of Chemical Physics, 2018, 149, 045103.	1.2	18
1067	Combining multi-scale modelling methods to decipher molecular motions of a branching sucrose from glycoside-hydrolase family 70. PLoS ONE, 2018, 13, e0201323.	1.1	4
1068	Molecular Modeling of Structures and Interaction of Human Corticotropin-Releasing Factor (CRF) Binding Protein and CRF Type-2 Receptor. Frontiers in Endocrinology, 2018, 9, 43.	1.5	5
1069	Tailoring the Variational Implicit Solvent Method for New Challenges: Biomolecular Recognition and Assembly. Frontiers in Molecular Biosciences, 2018, 5, 13.	1.6	6
1070	Macromolecular crowding and the importance of proper hydration for the structure and dynamics of protein solutions. Physical Chemistry Chemical Physics, 2018, 20, 19581-19594.	1.3	11
1071	Peptide-Induced DNA Condensation into Virus-Mimicking Nanostructures. ACS Applied Materials & Interfaces, 2018, 10, 24349-24360.	4.0	29
1072	Conformational analysis of replica exchange MD: Temperature-dependent Markov networks for FF amyloid peptides. Journal of Chemical Physics, 2018, 149, 072323.	1.2	7

#	ARTICLE	IF	CITATIONS
1073	Endpoint-restricted adiabatic free energy dynamics approach for the exploration of biomolecular conformational equilibria. <i>Journal of Chemical Physics</i> , 2018, 149, 072316.	1.2	11
1074	Anti-Correlation between the Dynamics of the Active Site Loop and C-Terminal Tail in Relation to the Homodimer Asymmetry of the Mouse Erythroid 5-Aminolevulinate Synthase. <i>International Journal of Molecular Sciences</i> , 2018, 19, 1899.	1.8	7
1075	Identification of Inhibitors Targeting Ferredoxin-NADP+ Reductase from the <i>Xanthomonas citri</i> subsp. <i>citri</i> Phytopathogenic Bacteria. <i>Molecules</i> , 2018, 23, 29.	1.7	6
1076	A Comparative Study of Human Saposins. <i>Molecules</i> , 2018, 23, 422.	1.7	7
1077	Molecular Modeling and Structural Stability of Wild-Type and Mutant CYP51 from <i>Leishmania major</i> : In Vitro and In Silico Analysis of a Laboratory Strain. <i>Molecules</i> , 2018, 23, 696.	1.7	10
1078	Valid molecular dynamics simulations of human hemoglobin require a surprisingly large box size. <i>ELife</i> , 2018, 7, .	2.8	63
1079	Electrostatic Tuning of the Ligand Binding Mechanism by Glu27 in Nitrophorin 7. <i>Scientific Reports</i> , 2018, 8, 10855.	1.6	4
1080	Oligomer Formation Propensities of Dimeric Bundle Peptides Correlate with Cell Penetration Abilities. <i>ACS Central Science</i> , 2018, 4, 885-893.	5.3	16
1081	Continuous Uptake or Saturation? Investigation of Concentration and Surface-Packing-Specific Hemin Interaction with Lipid Membranes. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7547-7554.	1.2	17
1082	Effects of ethanol on the secondary structure specific hydration properties of Chymotrypsin Inhibitor 2 in its folded and unfolded forms. <i>Molecular Simulation</i> , 2018, 44, 1278-1290.	0.9	2
1083	Atomistic simulations indicate the functional loop-to-coiled-coil transition in influenza hemagglutinin is not downhill. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E7905-E7913.	3.3	16
1084	Probing the role of proline 135 on the structure, stability, and cell proliferation activity of human acidic fibroblast growth factor. <i>Archives of Biochemistry and Biophysics</i> , 2018, 654, 115-125.	1.4	7
1085	In silico fragment-based drug design with SEED. <i>European Journal of Medicinal Chemistry</i> , 2018, 156, 907-917.	2.6	18
1086	Mapping the sensing spots of aerolysin for single oligonucleotides analysis. <i>Nature Communications</i> , 2018, 9, 2823.	5.8	60
1087	Probing key elements of teixobactin-lipid II interactions in membranes. <i>Chemical Science</i> , 2018, 9, 6997-7008.	3.7	21
1088	Electrostatic lock in the transport cycle of the multidrug resistance transporter EmrE. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E7502-E7511.	3.3	32
1089	Chloride Ion Transport by the <i>E. coli</i> CLC Cl ⁻ /H ⁺ Antiporter: A Combined Quantum-Mechanical and Molecular-Mechanical Study. <i>Frontiers in Chemistry</i> , 2018, 6, 62.	1.8	10
1090	Why Is a High Temperature Needed by <i>Thermus thermophilus</i> Argonaute During mRNA Silencing: A Theoretical Study. <i>Frontiers in Chemistry</i> , 2018, 6, 223.	1.8	9

#	ARTICLE	IF	CITATIONS
1091	pVEC hydrophobic N-terminus is critical for antibacterial activity. <i>Journal of Peptide Science</i> , 2018, 24, e3083.	0.8	15
1092	All-Atom Simulations Reveal How Single-Point Mutations Promote Serpin Misfolding. <i>Biophysical Journal</i> , 2018, 114, 2083-2094.	0.2	19
1093	The influence of flexibility on the spectroscopic properties for organic molecules in solution: A theoretical study applied to A3R polypeptide. <i>Journal of Molecular Liquids</i> , 2018, 263, 334-341.	2.3	13
1094	H-Aggregation Effects between π -Conjugated Chromophores in Cofacial Dimers and Trimers: Comparison of Theory and Single-Molecule Experiment. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6431-6441.	1.2	12
1095	p.R180C mutation of glycosyltransferase B leads to B subgroup, an <i>in vitro</i> and <i>in silico</i> study. <i>Vox Sanguinis</i> , 2018, 113, 476-484.	0.7	3
1096	Dimer Interface of the Human Serotonin Transporter and Effect of the Membrane Composition. <i>Scientific Reports</i> , 2018, 8, 5080.	1.6	32
1097	Identification and characterization of smallest pore-forming protein in the cell wall of pathogenic <i>Corynebacterium urealyticum</i> DSM 7109. <i>BMC Biochemistry</i> , 2018, 19, 3.	4.4	7
1098	Coupling between an electrostatic network and the Zn ²⁺ binding site modulates Hv1 activation. <i>Journal of General Physiology</i> , 2018, 150, 863-881.	0.9	19
1099	Revival of collective water structure and dynamics in reverse micelles brought about by protein encapsulation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22932-22945.	1.3	10
1100	Atomic resolution mechanism of ligand binding to a solvent inaccessible cavity in T4 lysozyme. <i>PLoS Computational Biology</i> , 2018, 14, e1006180.	1.5	58
1101	How Reactive are Druggable Cysteines in Protein Kinases?. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1935-1946.	2.5	44
1102	Rational Design of Thermostable Carbonic Anhydrase Mutants Using Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2018, 122, 8526-8536.	1.2	38
1103	Conformational Transitions of Melittin between Aqueous and Lipid Phases: Comparison of Simulations with Experiments. <i>Journal of Physical Chemistry B</i> , 2018, 122, 8698-8705.	1.2	9
1104	Damage and Failure of Axonal Microtubule under Extreme High Strain Rate: An In-Silico Molecular Dynamics Study. <i>Scientific Reports</i> , 2018, 8, 12260.	1.6	16
1105	Predicting structural and energetic changes in Met ^{aromatic} motifs on methionine oxidation to the sulfoxide and sulfone. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 23132-23141.	1.3	11
1106	Constructing atomic structural models into cryo-EM densities using molecular dynamics – Pros and cons. <i>Journal of Structural Biology</i> , 2018, 204, 319-328.	1.3	9
1107	All-Hydrocarbon Staples and Their Effect over Peptide Conformation under Different Force Fields. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 2015-2023.	2.5	9
1108	An Interface-Driven Design Strategy Yields a Novel, Corrugated Protein Architecture. <i>ACS Synthetic Biology</i> , 2018, 7, 2226-2235.	1.9	11

#	ARTICLE	IF	CITATIONS
1109	Phosphorylation promotes binding affinity of Rap-Raf complex by allosteric modulation of switch loop dynamics. <i>Scientific Reports</i> , 2018, 8, 12976.	1.6	10
1110	Entropic forces drive clustering and spatial localization of influenza A M2 during viral budding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E8595-E8603.	3.3	47
1111	Heterogeneity in Dynamics of Dioctadecyldimethylammonium Bromide Bilayers: Molecular Dynamics Simulation and Neutron Scattering Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 20419-20430.	1.5	15
1112	Peripheral Membrane Proteins Facilitate Nanoparticle Binding at Lipid Bilayer Interfaces. <i>Langmuir</i> , 2018, 34, 10793-10805.	1.6	24
1113	Mechanism for the Regulated Control of Bacterial Transcription Termination by a Universal Adaptor Protein. <i>Molecular Cell</i> , 2018, 71, 911-922.e4.	4.5	65
1114	Gating mechanism of the extracellular entry to the lipid pathway in a TMEM16 scramblase. <i>Nature Communications</i> , 2018, 9, 3251.	5.8	70
1115	Atomistic Insights into Cryptochrome Interprotein Interactions. <i>Biophysical Journal</i> , 2018, 115, 616-628.	0.2	11
1116	Molecular insights into the interactions of GF β 17 with the gram - and gram + bacterial lipid bilayers. <i>Journal of Cellular Biochemistry</i> , 2018, 119, 9205-9216.	1.2	11
1117	Effect of Asp122 Mutation on the Hydride Transfer in <i>E. coli</i> DHFR Demonstrates the Goldilocks of Enzyme Flexibility. <i>Journal of Physical Chemistry B</i> , 2018, 122, 8006-8017.	1.2	11
1118	TMC1 Forms the Pore of Mechanosensory Transduction Channels in Vertebrate Inner Ear Hair Cells. <i>Neuron</i> , 2018, 99, 736-753.e6.	3.8	250
1119	Self-Assembly Simulations of Classic Claudins '' Insights into the Pore Structure, Selectivity, and Higher Order Complexes. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7463-7474.	1.2	37
1120	Gibbs Free-Energy Gradient along the Path of Glucose Transport through Human Glucose Transporter 3. <i>ACS Chemical Neuroscience</i> , 2018, 9, 2815-2823.	1.7	13
1121	The Structural Basis of IKs Ion-Channel Activation: Mechanistic Insights from Molecular Simulations. <i>Biophysical Journal</i> , 2018, 114, 2584-2594.	0.2	23
1122	A 5-Enolpyruvylshikimate 3-Phosphate Synthase Functions as a Transcriptional Repressor in <i>Populus</i> . <i>Plant Cell</i> , 2018, 30, 1645-1660.	3.1	56
1123	Flexible selection of the solute region in replica exchange with solute tempering: Application to protein-folding simulations. <i>Journal of Chemical Physics</i> , 2018, 149, 072304.	1.2	75
1124	Computational study of HIV gp120 as a target for polyanionic entry inhibitors: Exploiting the V3 loop region. <i>PLoS ONE</i> , 2018, 13, e0190658.	1.1	9
1125	Glutamate and Glycine Binding to the NMDA Receptor. <i>Structure</i> , 2018, 26, 1035-1043.e2.	1.6	42
1126	A Funneled Conformational Landscape Governs Flavivirus Fusion Peptide Interaction with Lipid Membranes. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3920-3932.	2.3	9

#	ARTICLE	IF	CITATIONS
1127	Folding free energy landscapes of α -sheets with non-polarizable and polarizable CHARMM force fields. <i>Journal of Chemical Physics</i> , 2018, 149, 072317.	1.2	28
1128	Novel Intermolecular Surface Force Unveils the Driving Force of the Actomyosin System. , 2018, , 257-274.		1
1129	Gradual Crossover from Subdiffusion to Normal Diffusion: A Many-Body Effect in Protein Surface Water. <i>Physical Review Letters</i> , 2018, 120, 248101.	2.9	56
1130	Structure of the μ -opioid receptor-Gi protein complex. <i>Nature</i> , 2018, 558, 547-552.	13.7	527
1131	Broadly conserved Na ⁺ -binding site in the N-lobe of prokaryotic multidrug MATE transporters. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E6172-E6181.	3.3	25
1132	Thermodynamics of Conformational Transitions in a Disordered Protein Backbone Model. <i>Biophysical Journal</i> , 2018, 114, 2799-2810.	0.2	14
1133	Refinement of Peptide Conformational Ensembles by 2D IR Spectroscopy: Application to Ala-Ala-Ala. <i>Biophysical Journal</i> , 2018, 114, 2820-2832.	0.2	16
1134	Lanosterol Disrupts Aggregation of Human β -Crystallin by Binding to the Hydrophobic Dimerization Interface. <i>Journal of the American Chemical Society</i> , 2018, 140, 8479-8486.	6.6	42
1135	Molecular determination of claudin-15 organization and channel selectivity. <i>Journal of General Physiology</i> , 2018, 150, 949-968.	0.9	44
1136	A direct interaction of cholesterol with the dopamine transporter prevents its out-to-inward transition. <i>PLoS Computational Biology</i> , 2018, 14, e1005907.	1.5	81
1137	Evolution of chemokine receptors is driven by mutations in the sodium binding site. <i>PLoS Computational Biology</i> , 2018, 14, e1006209.	1.5	18
1138	Universal Implementation of a Residue-Specific Force Field Based on CMAP Potentials and Free Energy Decomposition. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4474-4486.	2.3	30
1139	Novel tumor necrosis factor- α (TNF- α) inhibitors from small molecule library screening for their therapeutic activity profiles against rheumatoid arthritis using target-driven approaches and binary QSAR models. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 2464-2476.	2.0	21
1140	Molecular modeling of neurological membrane proteins α from binding sites to synapses. <i>Neuroscience Letters</i> , 2019, 700, 38-49.	1.0	3
1141	Analysis Libraries for Molecular Trajectories: A Cross-Language Synopsis. <i>Methods in Molecular Biology</i> , 2019, 2022, 503-527.	0.4	1
1142	MxB Restricts HIV-1 by Targeting the Tri-hexamer Interface of the Viral Capsid. <i>Structure</i> , 2019, 27, 1234-1245.e5.	1.6	36
1143	Highly sensitive and selective detection of single-nucleotide polymorphisms using gold nanoparticle MutS enzymes and a micro cantilever resonator. <i>Talanta</i> , 2019, 205, 120154.	2.9	16
1144	Overcoming Challenging Substituent Perturbations with Multisite β -Dynamics: A Case Study Targeting β -Secretase 1. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4875-4880.	2.1	17

#	ARTICLE	IF	CITATIONS
1145	Lysosomal integral membrane protein-2 (LIMP-2/SCARB2) is involved in lysosomal cholesterol export. <i>Nature Communications</i> , 2019, 10, 3521.	5.8	99
1146	An Effective Electric Dipole Model for Voltage-induced Gating Mechanism of Lysenin. <i>Scientific Reports</i> , 2019, 9, 11440.	1.6	3
1147	The conduction pathway of potassium channels is water free under physiological conditions. <i>Science Advances</i> , 2019, 5, eaaw6756.	4.7	48
1148	Individual and combined effects of urea and trimethylamine N-oxide (TMAO) on protein structures. <i>Journal of Molecular Liquids</i> , 2019, 293, 111443.	2.3	8
1149	In Silico Reoptimization of Binding Affinity and Drug-Resistance Circumvention Ability in Kinase Inhibitors: A Case Study with RL-45 and Src Kinase. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6664-6672.	1.2	9
1150	Conformation space of a heterodimeric ABC exporter under turnover conditions. <i>Nature</i> , 2019, 571, 580-583.	13.7	185
1151	Magnesium interactions with a CX26 connexon in lipid bilayers. <i>Journal of Molecular Modeling</i> , 2019, 25, 232.	0.8	2
1152	Machine Learning Classification Model for Functional Binding Modes of TEM-1 β -Lactamase. <i>Frontiers in Molecular Biosciences</i> , 2019, 6, 47.	1.6	13
1153	Whole-Cell Models and Simulations in Molecular Detail. <i>Annual Review of Cell and Developmental Biology</i> , 2019, 35, 191-211.	4.0	47
1154	ACAP1 assembles into an unusual protein lattice for membrane deformation through multiple stages. <i>PLoS Computational Biology</i> , 2019, 15, e1007081.	1.5	2
1155	Inter-Active Site Communication Mediated by the Dimer Interface β -Sheet in the Half-the-Sites Enzyme, Thymidylate Synthase. <i>Biochemistry</i> , 2019, 58, 3302-3313.	1.2	9
1156	Structural underpinnings of Ric8A function as a G-protein β -subunit chaperone and guanine-nucleotide exchange factor. <i>Nature Communications</i> , 2019, 10, 3084.	5.8	22
1157	NMR Structural Analysis of Isolated Shaker Voltage-Sensing Domain in LPPG Micelles. <i>Biophysical Journal</i> , 2019, 117, 388-398.	0.2	3
1158	Quantifying the Stability of the Hydronium Ion in Organic Solvents With Molecular Dynamics Simulations. <i>Frontiers in Chemistry</i> , 2019, 7, 439.	1.8	13
1159	Modeling pH-Dependent NMR Chemical Shift Perturbations in Peptides. <i>Biophysical Journal</i> , 2019, 117, 258-268.	0.2	2
1160	Computational insight into hydrogen persulfide and a new additive model for chemical and biological simulations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15988-16004.	1.3	8
1161	Loading and release of anticancer drug from phosphorene as a template material with high efficient carrier: From vacuum to cell membrane. <i>Journal of Molecular Liquids</i> , 2019, 291, 111346.	2.3	26
1162	Molecular Computations of Preferential Interaction Coefficients of IgG1 Monoclonal Antibodies with Sorbitol, Sucrose, and Trehalose and the Impact of These Excipients on Aggregation and Viscosity. <i>Molecular Pharmaceutics</i> , 2019, 16, 3657-3664.	2.3	20

#	ARTICLE	IF	CITATIONS
1163	Structure and assembly of the mitochondrial membrane remodelling GTPase Mgm1. <i>Nature</i> , 2019, 571, 429-433.	13.7	86
1164	Molecular mechanism of setron-mediated inhibition of full-length 5-HT3A receptor. <i>Nature Communications</i> , 2019, 10, 3225.	5.8	42
1165	Structural basis for the multitasking nature of the potato virus Y coat protein. <i>Science Advances</i> , 2019, 5, eaaw3808.	4.7	61
1166	Cryptic pocket formation underlies allosteric modulator selectivity at muscarinic GPCRs. <i>Nature Communications</i> , 2019, 10, 3289.	5.8	47
1167	Hofmeister Effects on Peptide Amphiphile Nanofiber Self-Assembly. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7006-7013.	1.2	13
1168	Cholesterol Modulates Membrane Properties and the Interaction of gp41 Fusion Peptide To Promote Membrane Fusion. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7113-7122.	1.2	26
1169	Unusual Organization of I-BAR Proteins on Tubular and Vesicular Membranes. <i>Biophysical Journal</i> , 2019, 117, 553-562.	0.2	27
1170	Chemo-Mechanical Coupling in the Transport Cycle of a Heme ABC Transporter. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7270-7281.	1.2	6
1171	Temporin L and aurein 2.5 have identical conformations but subtly distinct membrane and antibacterial activities. <i>Scientific Reports</i> , 2019, 9, 10934.	1.6	22
1172	Histidine at position 462 determines the low quinine sensitivity of ether-activated K ^v channel superfamily member K _v 12.1. <i>British Journal of Pharmacology</i> , 2019, 176, 2708-2723.	2.7	2
1173	The Pore-Lipid Interface: Role of Amino-Acid Determinants of Lipophilic Access by Ivabradine to the hERG1 Pore Domain. <i>Molecular Pharmacology</i> , 2019, 96, 259-271.	1.0	24
1174	Discovery of new azoles with potent activity against <i>Candida</i> spp. and <i>Candida albicans</i> biofilms through virtual screening. <i>European Journal of Medicinal Chemistry</i> , 2019, 179, 634-648.	2.6	15
1175	Molecular Basis for Membrane Selectivity of Antimicrobial Peptide Pleurocidin in the Presence of Different Eukaryotic and Prokaryotic Model Membranes. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3262-3276.	2.5	22
1176	Molecular Dynamics Simulation of Pure <i>n</i> -Alkanes and Their Mixtures at Elevated Temperatures Using Atomistic and Coarse-Grained Force Fields. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6229-6243.	1.2	56
1177	Crystal structure of jumping spider rhodopsin-1 as a light sensitive GPCR. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 14547-14556.	3.3	48
1178	Smoothed stimulation by membrane sterols drives Hedgehog pathway activity. <i>Nature</i> , 2019, 571, 284-288.	13.7	154
1179	Antifungal screening and in silico mechanistic studies of an in-house azole library. <i>Chemical Biology and Drug Design</i> , 2019, 94, 1944-1955.	1.5	6
1180	Interfacial Aromatics Mediating Cation- π Interactions with Choline-Containing Lipids Can Contribute as Much to Peripheral Protein Affinity for Membranes as Aromatics Inserted below the Phosphates. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3972-3977.	2.1	24

#	ARTICLE	IF	CITATIONS
1181	Histone Octamer Structure Is Altered Early in ISW2 ATP-Dependent Nucleosome Remodeling. <i>Cell Reports</i> , 2019, 28, 282-294.e6.	2.9	20
1182	Accelerating Membrane Simulations with Hydrogen Mass Repartitioning. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4673-4686.	2.3	85
1183	Calculation of Conformational Free Energies with the Focused Confinement Method. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6760-6768.	2.3	4
1184	How Sugars Modify Caffeine Self-Association and Solubility: Resolving a Mechanism of Selective Hydrotrophy. <i>Journal of the American Chemical Society</i> , 2019, 141, 18056-18063.	6.6	20
1185	Insight into the Structure of the α -Unstructured τ Protein. <i>Structure</i> , 2019, 27, 1710-1715.e4.	1.6	39
1186	Large-scale conformational rearrangement of the ± 5 -helix of G_{\pm} subunits in complex with the guanine nucleotide exchange factor Ric8A. <i>Journal of Biological Chemistry</i> , 2019, 294, 17875-17882.	1.6	8
1187	Molecular Mechanism for Gramicidin Dimerization and Dissociation in Bilayers of Different Thickness. <i>Biophysical Journal</i> , 2019, 117, 1831-1844.	0.2	15
1188	A Molecular Mechanics Model for Flavins. <i>Journal of Computational Chemistry</i> , 2019, 40, 2834-2842.	1.5	18
1189	The Role of a Crystallographically Unresolved Cytoplasmic Loop in Stabilizing the Bacterial Membrane Insertase YidC2. <i>Scientific Reports</i> , 2019, 9, 14451.	1.6	9
1190	Spliceosomal Prp8 intein at the crossroads of protein and RNA splicing. <i>PLoS Biology</i> , 2019, 17, e3000104.	2.6	28
1191	String Method for Protein-Protein Binding Free-Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5829-5844.	2.3	33
1192	Structural basis for substrate specificity and regulation of nucleotide sugar transporters in the lipid bilayer. <i>Nature Communications</i> , 2019, 10, 4657.	5.8	23
1193	Topology, landscapes, and biomolecular energy transport. <i>Nature Communications</i> , 2019, 10, 4662.	5.8	8
1194	Transportin-1 binds to the HIV-1 capsid via a nuclear localization signal and triggers uncoating. <i>Nature Microbiology</i> , 2019, 4, 1840-1850.	5.9	76
1195	Prechondrogenic ATDC5 Cell Attachment and Differentiation on Graphene Foam; Modulation by Surface Functionalization with Fibronectin. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 41906-41924.	4.0	17
1196	Azi-medetomidine: Synthesis and Characterization of a Novel ± 2 Adrenergic Photoaffinity Ligand. <i>ACS Chemical Neuroscience</i> , 2019, 10, 4716-4728.	1.7	5
1197	Bases of Bacterial Sodium Channel Selectivity Among Organic Cations. <i>Scientific Reports</i> , 2019, 9, 15260.	1.6	7
1198	PEPCONF, a diverse data set of peptide conformational energies. <i>Scientific Data</i> , 2019, 6, 180310.	2.4	23

#	ARTICLE	IF	CITATIONS
1199	Dynamic modulation of the lipid translocation groove generates a conductive ion channel in Ca ²⁺ -bound nhTMEM16. <i>Nature Communications</i> , 2019, 10, 4972.	5.8	23
1200	How BamA recruits OMP substrates via poly-POTRA domain. <i>FASEB Journal</i> , 2019, 33, 14690-14702.	0.2	3
1201	Biochemical and Structural Insights Concerning Triclosan Resistance in a Novel YX7K Type Enoyl-Acyl Carrier Protein Reductase from Soil Metagenome. <i>Scientific Reports</i> , 2019, 9, 15401.	1.6	3
1202	A thiazole-derived oridonin analogue exhibits antitumor activity by directly and allosterically inhibiting STAT3. <i>Journal of Biological Chemistry</i> , 2019, 294, 17471-17486.	1.6	20
1203	Antileishmanial activity of terpenylquinones on <i>Leishmania infantum</i> and their effects on <i>Leishmania</i> topoisomerase IB. <i>International Journal for Parasitology: Drugs and Drug Resistance</i> , 2019, 11, 70-79.	1.4	22
1204	Crowder-Induced Conformational Ensemble Shift in <i>Escherichia coli</i> Prolyl-tRNA Synthetase. <i>Biophysical Journal</i> , 2019, 117, 1269-1284.	0.2	12
1205	Defective cell adhesion function of solute transporter, SLC4A11, in endothelial corneal dystrophies. <i>Human Molecular Genetics</i> , 2020, 29, 97-116.	1.4	18
1206	Polymer-like Model to Study the Dynamics of Dynamin Filaments on Deformable Membrane Tubes. <i>Biophysical Journal</i> , 2019, 117, 1870-1891.	0.2	13
1207	Study and Simulation of Nanoparticle Translocation Through Cell Membrane. <i>Iranian Journal of Science and Technology - Transactions of Mechanical Engineering</i> , 2019, , 1.	0.8	3
1208	Solubility of Caffeine in Supercritical CO ₂ : A Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry B</i> , 2019, 123, 9685-9691.	1.2	10
1209	Horizontal transfer of a pathway for coumarate catabolism unexpectedly inhibits purine nucleotide biosynthesis. <i>Molecular Microbiology</i> , 2019, 112, 1784-1797.	1.2	5
1210	Chirality-Dependent Adsorption between Amphipathic Peptide and POPC Membrane. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4760.	1.8	11
1211	The Effects of Calcium on Lipid-Protein Interactions and Ion Flux in the Cx26 Connexon Embedded into a POPC Bilayer. <i>Journal of Membrane Biology</i> , 2019, 252, 451-464.	1.0	3
1212	Force Fields for Small Molecules. <i>Methods in Molecular Biology</i> , 2019, 2022, 21-54.	0.4	29
1213	Applications of Molecular Dynamics Simulation in Structure Prediction of Peptides and Proteins. <i>Computational and Structural Biotechnology Journal</i> , 2019, 17, 1162-1170.	1.9	73
1214	Development and Validation of the Quantum Mechanical Bespoke Protein Force Field. <i>ACS Omega</i> , 2019, 4, 14537-14550.	1.6	18
1215	Structural and Functional Characterization of Dynamic Oligomerization in <i>Burkholderia cenocepacia</i> HMG-CoA Reductase. <i>Biochemistry</i> , 2019, 58, 3960-3970.	1.2	7
1216	Mechanisms of Nanonewton Mechanostability in a Protein Complex Revealed by Molecular Dynamics Simulations and Single-Molecule Force Spectroscopy. <i>Journal of the American Chemical Society</i> , 2019, 141, 14752-14763.	6.6	55

#	ARTICLE	IF	CITATIONS
1217	Specific inter-domain interactions stabilize a compact HIV-1 Gag conformation. <i>PLoS ONE</i> , 2019, 14, e0221256.	1.1	2
1218	Insights From Molecular Dynamics Simulations of a Number of G-Protein Coupled Receptor Targets for the Treatment of Pain and Opioid Use Disorders. <i>Frontiers in Molecular Neuroscience</i> , 2019, 12, 207.	1.4	19
1219	Stable calcium-free myocilin olfactomedin domain variants reveal challenges in differentiating between benign and glaucoma-causing mutations. <i>Journal of Biological Chemistry</i> , 2019, 294, 12717-12728.	1.6	13
1220	Broken force dispersal network in tip-links by the mutations at the Ca ²⁺ -binding residues induces hearing-loss. <i>Biochemical Journal</i> , 2019, 476, 2411-2425.	1.7	10
1221	Decreased conformational stability in the oncogenic N92I mutant of Ras-related C3 botulinum toxin substrate 1. <i>Science Advances</i> , 2019, 5, eaax1595.	4.7	6
1222	Combinatorial diversity of Syk recruitment driven by its multivalent engagement with Fc μ R1 β . <i>Molecular Biology of the Cell</i> , 2019, 30, 2331-2347.	0.9	11
1223	Structure-function guided modeling of chemokine-GPCR specificity for the chemokine XCL1 and its receptor XCR1. <i>Science Signaling</i> , 2019, 12, .	1.6	16
1224	An electrostatic switching mechanism to control the lipid transfer activity of Osh6p. <i>Nature Communications</i> , 2019, 10, 3926.	5.8	32
1225	Role of Fine Structural Dynamics in Recognition of Histone H3 by HP1 β (CSD) Dimer and Ability of Force Fields to Describe Their Interaction Network. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5659-5673.	2.3	2
1226	Cushing's syndrome driver mutation disrupts protein kinase A allosteric network, altering both regulation and substrate specificity. <i>Science Advances</i> , 2019, 5, eaaw9298.	4.7	43
1227	Antimicrobial peptide ROAD β 1 triggers phase change in local membrane environment to execute its activity. <i>Journal of Molecular Modeling</i> , 2019, 25, 281.	0.8	0
1228	Intestinal serotonin and fluoxetine exposure modulate bacterial colonization in the gut. <i>Nature Microbiology</i> , 2019, 4, 2064-2073.	5.9	264
1229	Surface Shear Viscosity and Interleaflet Friction from Nonequilibrium Simulations of Lipid Bilayers. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6471-6481.	2.3	27
1230	Structural Characterization of Agonist Binding to an A ₃ Adenosine Receptor through Biomolecular Simulations and Mutagenesis Experiments. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 8831-8846.	2.9	8
1231	Accelerating Rare Dissociative Processes in Biomolecules Using Selectively Scaled MD Simulations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5817-5828.	2.3	36
1232	Voltage-Dependent Profile Structures of a Kv-Channel via Time-Resolved Neutron Interferometry. <i>Biophysical Journal</i> , 2019, 117, 751-766.	0.2	3
1233	Principles of tRNA ^{Ala} Selection by Alanyl-tRNA Synthetase Based on the Critical G3 \cdot U70 Base Pair. <i>ACS Omega</i> , 2019, 4, 15539-15548.	1.6	7
1234	Validation of the Generalized Force Fields GAFF, CGenFF, OPLS-AA, and PRODRGFF by Testing Against Experimental Osmotic Coefficient Data for Small Drug-Like Molecules. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4239-4247.	2.5	26

#	ARTICLE	IF	CITATIONS
1235	Structure and Dynamics of Mono- vs. Doubly Lipidated Rab5 in Membranes. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4773.	1.8	6
1236	Conformation and Domain Movement Analysis of Human Matrix Metalloproteinase-2: Role of Associated Zn ²⁺ and Ca ²⁺ Ions. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4194.	1.8	5
1237	Absolute Free Energy of Binding Calculations for Macrophage Migration Inhibitory Factor in Complex with a Druglike Inhibitor. <i>Journal of Physical Chemistry B</i> , 2019, 123, 8675-8685.	1.2	17
1238	Inhibition Mechanisms of <i>Rhodococcus erythropolis</i> 2-Hydroxybiphenyl-2-sulfinate Desulfinatease (<i>DszB</i>). <i>Journal of Physical Chemistry B</i> , 2019, 123, 9054-9065.	1.2	4
1239	Structure and Dynamics of Spherical and Rodlike Alkyl Ethoxylate Surfactant Micelles Investigated Using NMR Relaxation and Atomistic Molecular Dynamics Simulations. <i>Langmuir</i> , 2019, 35, 13880-13892.	1.6	3
1240	Connecting wettability, topography, and chemistry in a simple lipid-montmorillonite system. <i>Journal of Colloid and Interface Science</i> , 2019, 555, 498-508.	5.0	7
1241	Systematic parameterization of lignin for the CHARMM force field. <i>Green Chemistry</i> , 2019, 21, 109-122.	4.6	51
1242	Mechanical unfolding of alpha- and beta-helical protein motifs. <i>Soft Matter</i> , 2019, 15, 1243-1252.	1.2	23
1243	Single-channel permeability and glycerol affinity of human aquaglyceroporin AQP3. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2019, 1861, 768-775.	1.4	20
1244	Vapor-Liquid Equilibrium Simulations of Hydrocarbons Using Molecular Dynamics with Long-Range Lennard-Jones Interactions. <i>Energy & Fuels</i> , 2019, 33, 848-858.	2.5	27
1245	Adaptive Partitioning QM/MM for Molecular Dynamics Simulations: 6. Proton Transport through a Biological Channel. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 892-905.	2.3	27
1246	Posttranscriptional spin labeling of RNA by tetrazine-based cycloaddition. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 1805-1808.	1.5	19
1247	Novel flavin-based fluorescent proteins with red-shifted emission bands: a computational study. <i>Photochemical and Photobiological Sciences</i> , 2019, 18, 177-189.	1.6	13
1248	Sterol A-ring plasticity in hedgehog protein cholesterolysis supports a primitive substrate selectivity mechanism. <i>Chemical Communications</i> , 2019, 55, 1829-1832.	2.2	10
1249	Potential off-target effects of beta-blockers on gut hormone receptors: In silico study including GUT-DOCK™ A web service for small-molecule docking. <i>PLoS ONE</i> , 2019, 14, e0210705.	1.1	12
1250	Molecular dynamics simulation of protein-mediated biomineralization of amorphous calcium carbonate. <i>RSC Advances</i> , 2019, 9, 1653-1663.	1.7	17
1251	Kinetic and thermodynamic insights into sodium ion translocation through the μ -opioid receptor from molecular dynamics and machine learning analysis. <i>PLoS Computational Biology</i> , 2019, 15, e1006689.	1.5	46
1252	Computational analyses, molecular dynamics, and mutagenesis studies of unprocessed form of [NiFe] hydrogenase reveal the role of disorder for efficient enzyme maturation. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2019, 1860, 325-340.	0.5	7

#	ARTICLE	IF	CITATIONS
1253	Speed up differential evolution for computationally expensive protein structure prediction problems. <i>Swarm and Evolutionary Computation</i> , 2019, 50, 100493.	4.5	16
1254	Dissecting the thermodynamic contributions of the charged residues in the membrane anchoring of Bcl-xl C-terminal domain. <i>Chemistry and Physics of Lipids</i> , 2019, 218, 112-124.	1.5	2
1255	Surface Binding Energy Landscapes Affect Phosphodiesterase Isoform-Specific Inhibitor Selectivity. <i>Computational and Structural Biotechnology Journal</i> , 2019, 17, 101-109.	1.9	7
1256	Kinetic and molecular dynamics study of inhibition and transglycosylation in <i>Hypocrea jecorina</i> family 3 β -glucosidases. <i>Journal of Biological Chemistry</i> , 2019, 294, 3169-3180.	1.6	5
1257	Integrated Approaches Toward High-Affinity Artificial Protein Binders Obtained via Computationally Simulated Epitopes for Protein Recognition. <i>Advanced Functional Materials</i> , 2019, 29, 1807332.	7.8	36
1258	Quantification of the Number of Adsorbed DNA Molecules on Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4837-4847.	1.5	63
1259	Fundamental limitations of the time-dependent Stokes shift for investigating protein hydration dynamics. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4435-4443.	1.3	7
1260	Molecular simulation of peptides coming of age: Accurate prediction of folding, dynamics and structures. <i>Archives of Biochemistry and Biophysics</i> , 2019, 664, 76-88.	1.4	23
1261	The Phospholamban Pentamer Alters Function of the Sarcoplasmic Reticulum Calcium Pump SERCA. <i>Biophysical Journal</i> , 2019, 116, 633-647.	0.2	30
1262	Simulations of Biomolecules in Electrolyte Solutions. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800163.	1.3	4
1263	Effect of protein-protein interactions and solvent viscosity on the rotational diffusion of proteins in crowded environments. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 876-883.	1.3	39
1264	A computational study toward the "personalized" activity of alternariol " Does it matter for safe food at individual level?. <i>Food and Chemical Toxicology</i> , 2019, 130, 199-206.	1.8	10
1265	New evidence for dual binding site inhibitors of acetylcholinesterase as improved drugs for treatment of Alzheimer's disease. <i>Neuropharmacology</i> , 2019, 155, 131-141.	2.0	67
1266	In silico chemical library screening and experimental validation of novel compounds with potential varroacide activities. <i>Pesticide Biochemistry and Physiology</i> , 2019, 160, 11-19.	1.6	11
1267	Interaction of SNARE Mimetic Peptides with Lipid bilayers: Effects of Secondary Structure, Bilayer Composition and Lipid Anchoring. <i>Scientific Reports</i> , 2019, 9, 7708.	1.6	9
1268	The four-helix bundle in cholinesterase dimers: Structural and energetic determinants of stability. <i>Chemico-Biological Interactions</i> , 2019, 309, 108699.	1.7	4
1269	Toward a Model for Activation of Orai Channel. <i>IScience</i> , 2019, 16, 356-367.	1.9	24
1270	Glycerol transport through the aquaglyceroporin GlpF: bridging dynamics and kinetics with atomic simulation. <i>Chemical Science</i> , 2019, 10, 6957-6965.	3.7	10

#	ARTICLE	IF	CITATIONS
1271	Expanding the range of binding energies and oxidizability of biologically relevant S ^α -aromatic interactions: imidazolium and phenolate binding to sulfoxide and sulfone. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14620-14628.	1.3	5
1272	Hydration dynamics of proteins in reverse micelles probed by ¹ H-NOESY/ ¹ H-ROESY NMR and ¹⁷ O-nuclear quadrupole resonance (NQR). <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14571-14582.	1.3	4
1273	Modeling of Specific Lipopolysaccharide Binding Sites on a Gram-Negative Porin. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5700-5708.	1.2	11
1274	Probing the transition state in enzyme catalysis by high-pressure NMR dynamics. <i>Nature Catalysis</i> , 2019, 2, 726-734.	16.1	30
1275	Comparative Exploratory Analysis of Intrinsically Disordered Protein Dynamics Using Machine Learning and Network Analytic Methods. <i>Frontiers in Molecular Biosciences</i> , 2019, 6, 42.	1.6	22
1276	Conformational transitions of a neurotensin receptor-Gi1 complex. <i>Nature</i> , 2019, 572, 80-85.	13.7	199
1277	Shaft Function of Kinesin-1 TM s $\hat{\pm}$ 4 Helix in the Processive Movement. <i>Cellular and Molecular Bioengineering</i> , 2019, 12, 345-354.	1.0	5
1278	Atomistic Simulations of Membrane Ion Channel Conduction, Gating, and Modulation. <i>Chemical Reviews</i> , 2019, 119, 7737-7832.	23.0	87
1279	Identification and functional analysis of missense mutations in the lecithin cholesterol acyltransferase gene in a Chilean patient with hypoalphalipoproteinemia. <i>Lipids in Health and Disease</i> , 2019, 18, 132.	1.2	7
1280	Interdigitation of Lipids Induced by Membrane-Active Proteins. <i>Journal of Membrane Biology</i> , 2019, 252, 331-342.	1.0	13
1281	Oxidation-induced destabilization of the fibrinogen α -C ₁ domain dimer investigated by molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 826-836.	1.5	13
1282	Understanding the stability of polypeptide membranes in ionic liquids: a theoretical molecular dynamics study. <i>New Journal of Chemistry</i> , 2019, 43, 10151-10161.	1.4	16
1283	Understanding the Role of Preferential Exclusion of Sugars and Polyols from Native State IgG1 Monoclonal Antibodies and its Effect on Aggregation and Reversible Self-Association. <i>Pharmaceutical Research</i> , 2019, 36, 109.	1.7	28
1284	Modulating Hinge Flexibility in the APP Transmembrane Domain Alters γ -Secretase Cleavage. <i>Biophysical Journal</i> , 2019, 116, 2103-2120.	0.2	34
1285	Use of Interaction Energies in QM/MM Free Energy Simulations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4632-4645.	2.3	21
1286	The solution structure of the human IgG2 subclass is distinct from those for human IgG1 and IgG4 providing an explanation for their discrete functions. <i>Journal of Biological Chemistry</i> , 2019, 294, 10789-10806.	1.6	14
1287	A Public BCR Present in a Unique Dual-Receptor-Expressing Lymphocyte from Type 1 Diabetes Patients Encodes a Potent T Cell Autoantigen. <i>Cell</i> , 2019, 177, 1583-1599.e16.	13.5	103
1288	Mechanism of Cardiac Troponin C Calcium Sensitivity Modulation by Small Molecules Illuminated by Umbrella Sampling Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2964-2972.	2.5	11

#	ARTICLE	IF	CITATIONS
1289	Structural comparison strengthens the higher-order classification of proteases related to chymotrypsin. <i>PLoS ONE</i> , 2019, 14, e0216659.	1.1	16
1290	Structures of the otopetrin proton channels Otop1 and Otop3. <i>Nature Structural and Molecular Biology</i> , 2019, 26, 518-525.	3.6	48
1291	Inward-facing conformation of a multidrug resistance MATE family transporter. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 12275-12284.	3.3	36
1292	The role of conserved arginine in the GH70 family: a computational study of the structural features and their implications on the catalytic mechanism of GTF-SI from <i>Streptococcus mutans</i> . <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 6269-6276.	1.5	7
1293	Chiral Inversion of Amino Acids in Antiparallel β -Sheets at Interfaces Probed by Vibrational Sum Frequency Generation Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5769-5781.	1.2	20
1294	The L46P Mutant Confers a Novel Allosteric Mechanism of Resistance Toward the Influenza A Virus M2 S31N Proton Channel Blockers. <i>Molecular Pharmacology</i> , 2019, 96, 148-157.	1.0	14
1295	Carbon nanotubes encapsulating fullerene as water nano-channels with distinctive selectivity: Molecular dynamics simulation. <i>Applied Surface Science</i> , 2019, 489, 198-209.	3.1	23
1296	Reduced level of docosahexaenoic acid shifts GPCR neuroreceptors to less ordered membrane regions. <i>PLoS Computational Biology</i> , 2019, 15, e1007033.	1.5	25
1297	PACKMOL-Memgen: A Simple-To-Use, Generalized Workflow for Membrane-Protein Lipid-Bilayer System Building. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2522-2528.	2.5	121
1298	Structural determinants for peptide-bond formation by asparaginyl ligases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 11737-11746.	3.3	81
1299	Interaction of Alt a 1 with SLC22A17 in the airway mucosa. <i>Allergy: European Journal of Allergy and Clinical Immunology</i> , 2019, 74, 2167-2180.	2.7	10
1300	DNA Conformational Changes Play a Force-Generating Role during Bacteriophage Genome Packaging. <i>Biophysical Journal</i> , 2019, 116, 2172-2180.	0.2	13
1301	Mechanistic insight into the early stages of amyloid formation using an anuran peptide. <i>Peptide Science</i> , 2019, 111, e24120.	1.0	12
1302	Paclitaxel interaction with cucurbit [7]uril and acyclic Cucurbit[4]uril nanocontainers: A computational approach. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 90, 210-218.	1.3	3
1303	Interaction of Mycotoxin Alternariol with Serum Albumin. <i>International Journal of Molecular Sciences</i> , 2019, 20, 2352.	1.8	39
1304	Hg-supported phospholipid monolayer as rapid screening device for low molecular weight narcotic compounds in water. <i>Analytica Chimica Acta</i> , 2019, 1069, 98-107.	2.6	5
1305	Ion and pH Sensitivity of a TMBIM Ca ²⁺ Channel. <i>Structure</i> , 2019, 27, 1013-1021.e3.	1.6	19
1306	<i>Salmonella</i> Membrane Structural Remodeling Increases Resistance to Antimicrobial Peptide LL-37. <i>ACS Infectious Diseases</i> , 2019, 5, 1214-1222.	1.8	35

#	ARTICLE	IF	CITATIONS
1307	Rotamer Dynamics: Analysis of Rotamers in Molecular Dynamics Simulations of Proteins. <i>Biophysical Journal</i> , 2019, 116, 2062-2072.	0.2	16
1308	Preferential Binding of Cytochrome <i>c</i> to Anionic Ligand-Coated Gold Nanoparticles: A Complementary Computational and Experimental Approach. <i>ACS Nano</i> , 2019, 13, 6856-6866.	7.3	31
1309	Molecular modeling studies on the interactions of 7-methoxytacrine-4-pyridinealoxime, 4-PA, 2-PAM, and obidoxime with VX-inhibited human acetylcholinesterase: a near attack conformation approach. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2019, 34, 1018-1029.	2.5	18
1310	Dynamical landscape in DODAB membrane system: MD simulation & neutron scattering studies. <i>Physica B: Condensed Matter</i> , 2019, 562, 55-58.	1.3	4
1311	Structural Investigation of Human Prolactin Receptor Transmembrane Domain Homodimerization in a Membrane Environment through Multiscale Simulations. <i>Journal of Physical Chemistry B</i> , 2019, 123, 4858-4866.	1.2	3
1312	Methods for the Refinement of Protein Structure 3D Models. <i>International Journal of Molecular Sciences</i> , 2019, 20, 2301.	1.8	44
1313	Structure and Dynamics of the Central Lipid Pool and Proteins of the Bacterial Holo-Translocon. <i>Biophysical Journal</i> , 2019, 116, 1931-1940.	0.2	22
1314	Applications of molecular modeling to flavoproteins: Insights and challenges. <i>Methods in Enzymology</i> , 2019, 620, 277-314.	0.4	9
1315	A Crucial Role for Side-Chain Conformation in the Versatile Charge Selectivity of Cys-Loop Receptors. <i>Biophysical Journal</i> , 2019, 116, 1667-1681.	0.2	2
1316	Molecular Insights on the Release of Avibactam from the Acyl-Enzyme Complex. <i>Biophysical Journal</i> , 2019, 116, 1650-1657.	0.2	8
1317	Computer-designed active human butyrylcholinesterase double mutant with a new catalytic triad. <i>Chemico-Biological Interactions</i> , 2019, 306, 138-146.	1.7	31
1318	Polarizable embedding for simulating redox potentials of biomolecules. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 11642-11650.	1.3	20
1319	Effects of Pressure and Temperature on the Atomic Fluctuations of Dihydrofolate Reductase from a Psychropiezophile and a Mesophile. <i>International Journal of Molecular Sciences</i> , 2019, 20, 1452.	1.8	9
1320	PhysNet: A Neural Network for Predicting Energies, Forces, Dipole Moments, and Partial Charges. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3678-3693.	2.3	501
1322	Structural basis for functional interactions in dimers of SLC26 transporters. <i>Nature Communications</i> , 2019, 10, 2032.	5.8	49
1323	Optimization and Evaluation of Site-Identification by Ligand Competitive Saturation (SILCS) as a Tool for Target-Based Ligand Optimization. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3018-3035.	2.5	47
1324	Synthesis, Biological Evaluation, and Molecular Modeling Studies of New Thiadiazole Derivatives as Potent P2X7 Receptor Inhibitors. <i>Frontiers in Chemistry</i> , 2019, 7, 261.	1.8	15
1325	Evolution of All-Atom Protein Force Fields to Improve Local and Global Properties. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2227-2234.	2.1	65

#	ARTICLE	IF	CITATIONS
1326	Structural insight into YcbB-mediated beta-lactam resistance in Escherichia coli. Nature Communications, 2019, 10, 1849.	5.8	29
1327	Unraveling Photocatalytic Mechanism and Selectivity in PET-RAFT Polymerization. Advanced Theory and Simulations, 2019, 2, 1900038.	1.3	32
1328	Conservation of conformational dynamics across prokaryotic actins. PLoS Computational Biology, 2019, 15, e1006683.	1.5	4
1329	Ligand retargeting by binding site analogy. European Journal of Medicinal Chemistry, 2019, 175, 107-113.	2.6	2
1330	Combining Structural Data with Computational Methodologies to Investigate Structure-Function Relationships in TRP Channels. Methods in Molecular Biology, 2019, 1987, 65-82.	0.4	5
1331	Multiconfigurational Coarse-Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2019, 15, 3306-3315.	2.3	22
1332	Chlorogenic acid isomers directly interact with Keap 1-Nrf2 signaling in Caco-2 cells. Molecular and Cellular Biochemistry, 2019, 457, 105-118.	1.4	42
1333	Molecular Dynamics Investigation into the Effect of Zinc(II) on the Structure and Membrane Interactions of the Antimicrobial Peptide Clavanin A. Journal of Physical Chemistry B, 2019, 123, 3163-3176.	1.2	18
1334	Free energy analysis of membrane pore formation process in the presence of multiple melittin peptides. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 1409-1419.	1.4	25
1335	Computational Models for Activated Human MEK1: Identification of Key Active Site Residues and Interactions. Journal of Chemical Information and Modeling, 2019, 59, 2383-2393.	2.5	4
1336	Effects of Selective Substitution of Cysteine Residues on the Conformational Properties of Chlorotoxin Explored by Molecular Dynamics Simulations. International Journal of Molecular Sciences, 2019, 20, 1261.	1.8	6
1337	MD Simulation Investigation on the Binding Process of Smoke-Derived Germination Stimulants to Its Receptor. Journal of Chemical Information and Modeling, 2019, 59, 1554-1562.	2.5	17
1338	How cardiolipin modulates the dynamics of respiratory complex I. Science Advances, 2019, 5, eaav1850.	4.7	56
1339	Conformational landscape alternations promote oncogenic activities of Ras-related C3 botulinum toxin substrate 1 as revealed by NMR. Science Advances, 2019, 5, eaav8945.	4.7	18
1340	Dimerization energetics of curli fiber subunits CsgA and CsgB. Npj Computational Materials, 2019, 5, .	3.5	11
1341	Probing the effects of nonannular lipid binding on the stability of the calcium pump SERCA. Scientific Reports, 2019, 9, 3349.	1.6	4
1342	Dynamic Studies on Intrinsically Disordered Regions of Two Paralogous Transcription Factors Reveal Rigid Segments with Important Biological Functions. Journal of Molecular Biology, 2019, 431, 1353-1369.	2.0	25
1343	Dynamics in Acetamide+LiNO3 Deep Eutectic Solvents. Physica B: Condensed Matter, 2019, 562, 13-16.	1.3	9

#	ARTICLE	IF	CITATIONS
1344	Extracellular gating of glucose transport through GLUT 1. <i>Biochemical and Biophysical Research Communications</i> , 2019, 511, 573-578.	1.0	10
1345	Can All-Atom Molecular Dynamics Simulations Quantitatively Describe Homeodomain-DNA Binding Equilibria?. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2635-2648.	2.3	8
1346	U-shaped caveolin-1 conformations are tightly regulated by hydrogen bonds with lipids. <i>Journal of Computational Chemistry</i> , 2019, 40, 1570-1577.	1.5	8
1347	Discovering Monoterpene Catalysis Inside Nanocapsules with Multiscale Modeling and Experiments. <i>Journal of the American Chemical Society</i> , 2019, 141, 6234-6246.	6.6	42
1348	Myoglobinopathy is an adult-onset autosomal dominant myopathy with characteristic sarcoplasmic inclusions. <i>Nature Communications</i> , 2019, 10, 1396.	5.8	11
1349	Towards capturing cellular complexity: combining encapsulation and macromolecular crowding in a reverse micelle. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8108-8120.	1.3	7
1350	ATP-Dependent Signaling in Simulations of a Revised Model of Cystic Fibrosis Transmembrane Conductance Regulator (CFTR). <i>Journal of Physical Chemistry B</i> , 2019, 123, 3177-3188.	1.2	4
1351	Molecular Modeling Investigation of the Interaction between <i>Humicola insolens</i> Cutinase and SDS Surfactant Suggests a Mechanism for Enzyme Inactivation. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 1977-1987.	2.5	14
1352	Oriental and Folding Thermodynamics via Electric Dipole Moment Restraining. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2599-2608.	1.2	5
1353	Molecular insight into the wetting behavior and amphiphilic character of cellulose nanocrystals. <i>Advances in Colloid and Interface Science</i> , 2019, 267, 15-25.	7.0	45
1354	Interpretation of spectroscopic data using molecular simulations for the secondary active transporter BetP. <i>Journal of General Physiology</i> , 2019, 151, 381-394.	0.9	7
1355	Insights into water accessible pathways and the inactivation mechanism of proton translocation by the membrane-embedded domain of V-type ATPases. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2019, 1861, 1004-1010.	1.4	10
1356	A Dynamic Hydrophobic Core and Surface Salt Bridges Thermostabilize a Designed Three-Helix Bundle. <i>Biophysical Journal</i> , 2019, 116, 621-632.	0.2	16
1357	Adaptations for pressure and temperature effects on loop motion in <i>Escherichia coli</i> and <i>Moritella profunda</i> dihydrofolate reductase. <i>High Pressure Research</i> , 2019, 39, 225-237.	0.4	6
1358	Exploration of Catalytic Selectivity for Aminotransferase (BtrR) Based on Multiple Molecular Dynamics Simulations. <i>International Journal of Molecular Sciences</i> , 2019, 20, 1188.	1.8	5
1359	Computational modeling of the adsorption of capping agent biomolecules to inorganic nanoparticles. , 2019, , 21-41.		0
1360	Statistical properties for diffusive motion of hydration water on protein surface. <i>Physica B: Condensed Matter</i> , 2019, 562, 1-5.	1.3	2
1361	Evaluating Unexpectedly Short Non-covalent Distances in X-ray Crystal Structures of Proteins with Electronic Structure Analysis. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2199-2211.	2.5	38

#	ARTICLE	IF	CITATIONS
1363	Molecular Dynamics Simulations of the Allosteric Modulation of the Adenosine A2a Receptor by a Mini-G Protein. <i>Scientific Reports</i> , 2019, 9, 5495.	1.6	13
1364	Estimation of the breadth of CD4bs targeting HIV antibodies by molecular modeling and machine learning. <i>PLoS Computational Biology</i> , 2019, 15, e1006954.	1.5	16
1365	Exposing the Interplay Between Enzyme Turnover, Protein Dynamics, and the Membrane Environment in Monoamine Oxidase B. <i>Biochemistry</i> , 2019, 58, 2362-2372.	1.2	12
1366	Assessment of Conformational State Transitions of Class B GPCRs Using Molecular Dynamics. <i>Methods in Molecular Biology</i> , 2019, 1947, 3-19.	0.4	3
1367	Active-Site Heterogeneity of Lactate Dehydrogenase. <i>ACS Catalysis</i> , 2019, 9, 4236-4246.	5.5	10
1368	Molecular Dynamics-Decorated Finite Element Method (MDeFEM): Application to the Gating Mechanism of Mechanosensitive Channels. , 2019, , 77-128.		0
1369	Importance of the Force Field Choice in Capturing Functionally Relevant Dynamics in the von Willebrand Factor. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1928-1934.	2.1	32
1370	The Disulfide Bond between Cys22 and Cys27 in the Protease Domain Modulate Clotting Activity of Coagulation Factor X. <i>Thrombosis and Haemostasis</i> , 2019, 119, 871-881.	1.8	6
1371	Increased H-Bond Stability Relates to Altered β -Cleavage Efficiency and A β Levels in the I45T Familial Alzheimer's Disease Mutant of APP. <i>Scientific Reports</i> , 2019, 9, 5321.	1.6	20
1372	The human adenovirus type 5 E1B 55kDa protein interacts with RNA promoting timely DNA replication and viral late mRNA metabolism. <i>PLoS ONE</i> , 2019, 14, e0214882.	1.1	4
1373	Structural Conservation of the Two Phosphoinositide-Binding Sites in WIPI Proteins. <i>Journal of Molecular Biology</i> , 2019, 431, 1494-1505.	2.0	31
1374	Structure of Outward-Facing PglK and Molecular Dynamics of Lipid-Linked Oligosaccharide Recognition and Translocation. <i>Structure</i> , 2019, 27, 669-678.e5.	1.6	29
1375	Self-Assembled Cationic β -Cyclodextrin Nanostructures for siRNA Delivery. <i>Molecular Pharmaceutics</i> , 2019, 16, 1358-1366.	2.3	47
1376	Directionality of dynein is controlled by the angle and length of its stalk. <i>Nature</i> , 2019, 566, 407-410.	13.7	50
1377	Dynamic Landscape in Self-Assembled Surfactant Aggregates. <i>Langmuir</i> , 2019, 35, 14151-14172.	1.6	30
1378	Modulation of Human Hsp90 α Conformational Dynamics by Allosteric Ligand Interaction at the C-Terminal Domain. <i>Scientific Reports</i> , 2019, 9, 1600.	1.6	27
1379	Minor sequence modifications in temporin B cause drastic changes in antibacterial potency and selectivity by fundamentally altering membrane activity. <i>Scientific Reports</i> , 2019, 9, 1385.	1.6	26
1380	Three distinct regions of cRaf kinase domain interact with membrane. <i>Scientific Reports</i> , 2019, 9, 2057.	1.6	9

#	ARTICLE	IF	CITATIONS
1381	Transport of cystine across xCâ” antiporter. Archives of Biochemistry and Biophysics, 2019, 664, 117-126.	1.4	10
1382	Quantifying correlations between mutational sites in the catalytic subunit of Î³-secretase. Journal of Molecular Graphics and Modelling, 2019, 88, 221-227.	1.3	4
1383	Modeling MesoBioNano systems with MBN Studio made easy. Journal of Molecular Graphics and Modelling, 2019, 88, 247-260.	1.3	34
1384	Anharmonic Vibrational Analysis of Biomolecules and Solvated Molecules Using Hybrid QM/MM Computations. Journal of Chemical Theory and Computation, 2019, 15, 1924-1938.	2.3	30
1385	A molecular mechanism for transthyretin amyloidogenesis. Nature Communications, 2019, 10, 925.	5.8	92
1386	Metal binding to the dynamic cytoplasmic domain of the cation diffusion facilitator (CDF) protein MamM induces a “locked” configuration. FEBS Journal, 2019, 286, 2193-2215.	2.2	9
1387	Characterization, Dynamics, and Mechanism of CXCR4 Antagonists on a Constitutively Active Mutant. Cell Chemical Biology, 2019, 26, 662-673.e7.	2.5	20
1388	Equilibrium properties of protic ionic liquids based on metil-2-hydroxyethylammonium cation. Journal of Molecular Liquids, 2019, 282, 226-234.	2.3	3
1389	Graphene quantum dot assisted translocation of drugs into a cell membrane. Nanoscale, 2019, 11, 4503-4514.	2.8	56
1390	Changes in Microenvironment Modulate the B- to A-DNA Transition. Journal of Chemical Information and Modeling, 2019, 59, 2324-2330.	2.5	11
1391	A lipid gating mechanism for the channel-forming O antigen ABC transporter. Nature Communications, 2019, 10, 824.	5.8	44
1392	Influence of nanotube section on carboplatin confinement. Journal of Molecular Modeling, 2019, 25, 72.	0.8	7
1393	Crystal Structure and Conformational Dynamics of <i>Pyrococcus furiosus</i> Prolyl Oligopeptidase. Biochemistry, 2019, 58, 1616-1626.	1.2	19
1394	Adsorption of amino acids on graphene: assessment of current force fields. Soft Matter, 2019, 15, 2359-2372.	1.2	24
1395	Comparative Analysis of Protein Hydration from MD simulations with Additive and Polarizable Force Fields. Advanced Theory and Simulations, 2019, 2, 1800106.	1.3	22
1396	Biochemical, Kinetic, and Computational Structural Characterization of Shikimate Kinase from Methicillin-Resistant <i>Staphylococcus aureus</i> . Molecular Biotechnology, 2019, 61, 274-285.	1.3	5
1397	Ranking Reversible Covalent Drugs: From Free Energy Perturbation to Fragment Docking. Journal of Chemical Information and Modeling, 2019, 59, 2093-2102.	2.5	35
1398	Site-specific ubiquitylation and SUMOylation using genetic-code expansion and sortase. Nature Chemical Biology, 2019, 15, 276-284.	3.9	96

#	ARTICLE	IF	CITATIONS
1399	Dynamical Behavior of β -Lactamases and Penicillin-Binding Proteins in Different Functional States and Its Potential Role in Evolution. <i>Entropy</i> , 2019, 21, 1130.	1.1	7
1400	An experiment-informed signal transduction model for the role of the <i>Staphylococcus aureus</i> MecR1 protein in β -lactam resistance. <i>Scientific Reports</i> , 2019, 9, 19558.	1.6	11
1401	Molecular dynamics simulations suggest stabilizing mutations in a de novo designed β -sheet protein. <i>Protein Engineering, Design and Selection</i> , 2019, 32, 317-329.	1.0	6
1402	Clustering of atomic displacement parameters in bovine trypsin reveals a distributed lattice of atoms with shared chemical properties. <i>Scientific Reports</i> , 2019, 9, 19281.	1.6	7
1403	Allosteric response to ligand binding: Molecular dynamics study of the N-terminal domains in IP ₃ receptor. <i>Biophysics and Physicobiology</i> , 2019, 16, 232-239.	0.5	7
1405	Minor Chemistry Changes Alter Surface Hydration to Control Fibronectin Adsorption and Assembly into Nanofibrils. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900169.	1.3	8
1406	Calculating the Effect of Membrane Thickness on the Lifetime of the Gramicidin A Channel: A Landmark. <i>Biophysical Journal</i> , 2019, 117, 1779-1780.	0.2	0
1407	Molecular Oxygen Binding in the Mitochondrial Electron Transfer Flavoprotein. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4868-4879.	2.5	12
1408	Catalytic Mechanism of Aryl-Ether Bond Cleavage in Lignin by LigF and LigG. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10142-10151.	1.2	8
1409	Computational insights into lipid assisted peptide misfolding and aggregation in neurodegeneration. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22679-22694.	1.3	14
1410	Experimental and computational studies of noncovalent interactions in the metal-free ternary Lys-ATP system. <i>New Journal of Chemistry</i> , 2019, 43, 16898-16906.	1.4	4
1411	Computational screening of nanoparticles coupling to A β 40 peptides and fibrils. <i>Scientific Reports</i> , 2019, 9, 17804.	1.6	10
1412	A3 adenosine receptor activation mechanisms: molecular dynamics analysis of inactive, active, and fully active states. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 33, 983-996.	1.3	10
1413	Rational discovery of antimetastatic agents targeting the intrinsically disordered region of MBD2. <i>Science Advances</i> , 2019, 5, eaav9810.	4.7	21
1414	Lipid Interactions of a Ciliary Membrane TRP Channel: Simulation and Structural Studies of Polycystin-2. <i>Structure</i> , 2020, 28, 169-184.e5.	1.6	37
1415	A Molecular Dynamics Perspective To Identify Precursors to Aggregation in Human β -Crystallin Unravels the Mechanism of Childhood Cataracts. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10384-10393.	1.2	8
1416	Early Photocycle of Slr1694 Blue-Light Using Flavin Photoreceptor Unraveled through Adiabatic Excited-State Quantum Mechanical/Molecular Mechanical Dynamics. <i>Journal of the American Chemical Society</i> , 2019, 141, 20470-20479.	6.6	33
1417	Extensive free-energy simulations identify water as the base in nucleotide addition by DNA polymerase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 25048-25056.	3.3	20

#	ARTICLE	IF	CITATIONS
1418	Heteroaryldihydropyrimidines Alter Capsid Assembly By Adjusting the Binding Affinity and Pattern of the Hepatitis B Virus Core Protein. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 5104-5110.	2.5	15
1419	HKT1;5 Transporter Gene Expression and Association of Amino Acid Substitutions With Salt Tolerance Across Rice Genotypes. <i>Frontiers in Plant Science</i> , 2019, 10, 1420.	1.7	43
1420	Next-Generation Sequencing Reveals Novel Genetic Variants (SRY, DMRT1, NR5A1, DHH, DHX37) in Adults With 46,XY DSD. <i>Journal of the Endocrine Society</i> , 2019, 3, 2341-2360.	0.1	46
1421	On the Stability of the Water-Soluble Chlorophyll-Binding Protein (WSCP) Studied by Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10594-10604.	1.2	8
1422	Single-molecule sensing of peptides and nucleic acids by engineered aerolysin nanopores. <i>Nature Communications</i> , 2019, 10, 4918.	5.8	74
1423	The allosteric mechanism of substrate-specific transport in SLC6 is mediated by a volumetric sensor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 15947-15956.	3.3	23
1424	Planarity and out-of-plane vibrational modes of tryptophan and tyrosine in biomolecular modeling. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23943-23965.	1.3	4
1425	Non-detergent isolation of a cyanobacterial photosystem I using styrene maleic acid alternating copolymers. <i>RSC Advances</i> , 2019, 9, 31781-31796.	1.7	19
1426	In silico study on identification of novel MALT1 allosteric inhibitors. <i>RSC Advances</i> , 2019, 9, 39338-39347.	1.7	5
1427	Changes in protein hydration dynamics by encapsulation or crowding of ubiquitin: strong correlation between time-dependent Stokes shift and intermolecular nuclear Overhauser effect. <i>RSC Advances</i> , 2019, 9, 36982-36993.	1.7	5
1428	A model for dinitrogen binding in the E ₄ state of nitrogenase. <i>Chemical Science</i> , 2019, 10, 11110-11124.	3.7	48
1429	Assembly of Spinach Chloroplast ATP Synthase Rotor Ring Protein-Lipid Complex. <i>Frontiers in Molecular Biosciences</i> , 2019, 6, 135.	1.6	7
1430	20. Multiscale modeling of lipid membrane. , 2019, , 569-602.		0
1431	An activating mutation of the NSD2 histone methyltransferase drives oncogenic reprogramming in acute lymphocytic leukemia. <i>Oncogene</i> , 2019, 38, 671-686.	2.6	39
1432	The lipid environment determines the activity of the <i>Escherichia coli</i> ammonium transporter AmtB. <i>FASEB Journal</i> , 2019, 33, 1989-1999.	0.2	28
1433	Exploring protein-protein interactions using the site identification by ligand competitive saturation methodology. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 289-301.	1.5	21
1434	State-dependent Lipid Interactions with the A2a Receptor Revealed by MD Simulations Using In Vivo-Mimetic Membranes. <i>Structure</i> , 2019, 27, 392-403.e3.	1.6	80
1435	Electron-Coupled Double Proton Transfer in the Slr1694 BLUF Photoreceptor: A Multireference Electronic Structure Study. <i>Journal of Physical Chemistry B</i> , 2019, 123, 439-447.	1.2	23

#	ARTICLE	IF	CITATIONS
1436	Engineering of serine protease for improved thermostability and catalytic activity using rational design. <i>International Journal of Biological Macromolecules</i> , 2019, 126, 229-237.	3.6	47
1437	Cation- π Interactions between Methylated Ammonium Groups and Tryptophan in the CHARMM36 Additive Force Field. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 7-12.	2.3	58
1438	Highly tumor-specific DNA nanostructures discovered by in vivo screening of a nucleic acid cage library and their applications in tumor-targeted drug delivery. <i>Biomaterials</i> , 2019, 195, 1-12.	5.7	44
1439	Design and in Vivo Characterization of A ₁ Adenosine Receptor Agonists in the Native Ribose and Conformationally Constrained (N)-Methanocarba Series. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 1502-1522.	2.9	22
1440	Dynamic ion pair behavior stabilizes single α -helices in proteins. <i>Journal of Biological Chemistry</i> , 2019, 294, 3219-3234.	1.6	12
1441	H-NS uses an autoinhibitory conformational switch for environment-controlled gene silencing. <i>Nucleic Acids Research</i> , 2019, 47, 2666-2680.	6.5	45
1442	A NCAPG2-Derived Phosphopeptide Selectively Binds to the Polo-Box Domain of PLK1 and Inhibits Cancer Cell Proliferation. <i>International Journal of Peptide Research and Therapeutics</i> , 2019, 25, 1397-1403.	0.9	0
1443	Structural characterization and molecular dynamics simulations of the caprine and bovine solute carrier family 11 A1 (SLC11A1). <i>Journal of Computer-Aided Molecular Design</i> , 2019, 33, 265-285.	1.3	5
1444	Bidirectional Control of Autophagy by BECN1 BARA Domain Dynamics. <i>Molecular Cell</i> , 2019, 73, 339-353.e6.	4.5	61
1445	Gating and inactivation of mechanosensitive channels of small conductance: A continuum mechanics study. <i>Journal of the Mechanical Behavior of Biomedical Materials</i> , 2019, 90, 502-514.	1.5	2
1446	Specific Ion Effects on an Oligopeptide: Bidentate Binding Matters for the Guanidinium Cation. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 332-337.	7.2	10
1447	Spezifische Ionen-Effekte am Beispiel eines Oligopeptids: die Rolle zweizÄhniger Koordination beim Guanidinium-Kation. <i>Angewandte Chemie</i> , 2019, 131, 338-343.	1.6	0
1448	Atomistic insights into cardiolipin binding sites of cytochrome c oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2019, 1860, 224-232.	0.5	15
1449	Molecular dynamics simulations of macromolecular crystals. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019, 9, e1402.	6.2	25
1450	Lipid composition and salt concentration as regulatory factors of the anion selectivity of VDAC studied by coarse-grained molecular dynamics simulations. <i>Chemistry and Physics of Lipids</i> , 2019, 220, 66-76.	1.5	6
1451	Allosteric Control of <i>N</i> -Acetyl-Aspartate Hydrolysis by the Y231C and F295S Mutants of Human Aspartoacylase. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2299-2308.	2.5	6
1452	Improved Modeling of Halogenated Ligand-Protein Interactions Using the Drude Polarizable and CHARMM Additive Empirical Force Fields. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 215-228.	2.5	23
1453	AMBER and CHARMM Force Fields Inconsistently Portray the Microscopic Details of Phosphorylation. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 665-679.	2.3	18

#	ARTICLE	IF	CITATIONS
1454	On identifying collective displacements in apo-proteins that reveal eventual binding pathways. PLoS Computational Biology, 2019, 15, e1006665.	1.5	11
1455	A time and memory efficient recipe for fast normal mode computations of complexes with icosahedral symmetry. Journal of Molecular Graphics and Modelling, 2019, 87, 30-40.	1.3	3
1456	A molecular dynamics study on the role of the protonation state in the biosynthesis of R-PAC by AHAS. Chemical Physics Letters, 2019, 716, 247-251.	1.2	4
1457	Natural payload delivery of the doxorubicin anticancer drug from boron nitride oxide nanosheets. Applied Surface Science, 2019, 475, 666-675.	3.1	42
1458	Drug-induced diabetes type 2: In silico study involving class B GPCRs. PLoS ONE, 2019, 14, e0208892.	1.1	20
1459	Apolipoprotein A1 Forms 5/5 and 5/4 Antiparallel Dimers in Human High-density Lipoprotein. Molecular and Cellular Proteomics, 2019, 18, 854a-864.	2.5	17
1460	Membrane cholesterol depletion reduces downstream signaling activity of the adenosine A2A receptor. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 760-767.	1.4	44
1461	Molecular Mechanisms of Macular Degeneration Associated with the Complement Factor H Y402H Mutation. Biophysical Journal, 2019, 116, 215-226.	0.2	8
1462	Nanobody interaction unveils structure, dynamics and proteotoxicity of the Finnish-type amyloidogenic gelsolin variant. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2019, 1865, 648-660.	1.8	21
1463	Crystal Structure of the Human Cannabinoid Receptor CB2. Cell, 2019, 176, 459-467.e13.	13.5	268
1464	Developments and Applications of Coil-Library-Based Residue-Specific Force Fields for Molecular Dynamics Simulations of Peptides and Proteins. Journal of Chemical Theory and Computation, 2019, 15, 2761-2773.	2.3	11
1465	Role of Conformational Flexibility in Monte Carlo Simulations of Many-Protein Systems. Journal of Chemical Theory and Computation, 2019, 15, 1399-1408.	2.3	6
1466	Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of A β 22 Dimer. Journal of Chemical Theory and Computation, 2019, 15, 1440-1452.	2.3	102
1467	Dynamical Effects of Trimethylamine N-Oxide on Aqueous Solutions of Urea. Journal of Physical Chemistry B, 2019, 123, 1108-1115.	1.2	18
1468	Engineered Histidine-Enriched Facial Lipopeptides for Enhanced Intracellular Delivery of Functional siRNA to Triple Negative Breast Cancer Cells. ACS Applied Materials & Interfaces, 2019, 11, 4719-4736.	4.0	20
1469	Lipid-Dependent Alternating Access Mechanism of a Bacterial Multidrug ABC Exporter. ACS Central Science, 2019, 5, 43-56.	5.3	35
1470	Shifts in the selectivity filter dynamics cause modal gating in K ⁺ channels. Nature Communications, 2019, 10, 123.	5.8	66
1471	Structural Insights into Phylloquinone (Vitamin K1), Menaquinone (MK4, MK7), and Menadione (Vitamin T) Tj ETQq1 1.0.784314 rgBT / Dv	1.7	20

#	ARTICLE	IF	CITATIONS
1472	Acceleration of cryo-EM Flexible Fitting for Large Biomolecular Systems by Efficient Space Partitioning. <i>Structure</i> , 2019, 27, 161-174.e3.	1.6	16
1473	A brief appraisal of computational modeling of antimicrobial peptides' activity. <i>Drug Development Research</i> , 2019, 80, 28-32.	1.4	12
1474	Effect of solvation water shells on enzyme active sites in zinc-dependent hydrolases. <i>Structural Chemistry</i> , 2019, 30, 481-488.	1.0	4
1475	ORAI1 channel gating and selectivity is differentially altered by natural mutations in the first or third transmembrane domain. <i>Journal of Physiology</i> , 2019, 597, 561-582.	1.3	37
1476	Origin and Prediction of Highly Specific Bond Cleavage Sites in the Thermal Activation of Intact Protein Ions. <i>Chemistry - A European Journal</i> , 2019, 25, 823-834.	1.7	6
1477	Disulfide bridge formation influences ligand recognition by the ATAD2 bromodomain. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 157-167.	1.5	9
1478	Structural Characterization of Biomolecules through Atomistic Simulations Guided by DEER Measurements. <i>Structure</i> , 2019, 27, 359-370.e12.	1.6	20
1479	Activity and Thermostability of GH5 Endoglucanase Chimeras from Mesophilic and Thermophilic Parents. <i>Applied and Environmental Microbiology</i> , 2019, 85, .	1.4	28
1480	Force field development phase II: Relaxation of physics-based criteria or inclusion of more rigorous physics into the representation of molecular energetics. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 33, 205-264.	1.3	47
1481	Recognition and stabilization of geranylgeranylated human Rab5 by the GDP Dissociation Inhibitor (GDI). <i>Small GTPases</i> , 2019, 10, 227-242.	0.7	4
1482	6-Methyluracil derivatives as peripheral site ligand-hydroxamic acid conjugates: Reactivation for paraoxon-inhibited acetylcholinesterase. <i>European Journal of Medicinal Chemistry</i> , 2020, 185, 111787.	2.6	9
1483	Comprehensive structural modeling and preparation of human 5-HT _{2A} protein coupled receptor in functionally active form. <i>Biopolymers</i> , 2020, 111, e23329.	1.2	8
1484	Improved Modeling of Cation- π and Anion- π Ring Interactions Using the Drude Polarizable Empirical Force Field for Proteins. <i>Journal of Computational Chemistry</i> , 2020, 41, 439-448.	1.5	27
1485	Protein Nanotechnology. <i>Methods in Molecular Biology</i> , 2020, , .	0.4	4
1486	Binding mode of Pyridoclastox to myeloid cell leukemia-1 (Mcl-1) revealed by nuclear magnetic resonance spectroscopy, docking and molecular dynamics approaches. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 4162-4178.	2.0	4
1487	New strategy for identifying potential natural HIV-1 non-nucleoside reverse transcriptase inhibitors against drug-resistance: an in silico study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 3327-3341.	2.0	13
1488	Glycosylation effects on the structure and dynamics of a full-length Cel7A cellulase. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2020, 1868, 140248.	1.1	7
1489	The 3A6-TCR/superagonist/HLA-DR2a complex shows similar interface and reduced flexibility compared to the complex with self-peptide. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020, 88, 31-46.	1.5	0

#	ARTICLE	IF	CITATIONS
1490	Discovering the chloride pathway in the CFTR channel. Cellular and Molecular Life Sciences, 2020, 77, 765-778.	2.4	14
1491	Benserazide Perturbs Kif15â€kinesin Binding Protein Interaction with Prolonged Metaphase and Defects in Chromosomal Congestion: A Study Based on in silico Modeling and Cell Culture. Molecular Informatics, 2020, 39, 1900035.	1.4	6
1492	An experimental and computational study of the effect of aqueous solution on the multiphoton ionisation photoelectron spectrum of phenol. Faraday Discussions, 2019, 221, 202-218.	1.6	7
1493	Presence of substrate aids lateral gate separation in LptD. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183025.	1.4	17
1494	Substrate binding to Src: A new perspective on tyrosine kinase substrate recognition from NMR and molecular dynamics. Protein Science, 2020, 29, 350-359.	3.1	9
1495	Molecular dynamics study of membrane permeabilization by wild-type and mutant lytic peptides from the non-enveloped Flock House virus. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183102.	1.4	8
1496	Ligand-induced disorder-to-order transitions characterized by structural proteomics and molecular dynamics simulations. Journal of Proteomics, 2020, 211, 103544.	1.2	10
1497	Preparation of ternary photocatalysts and their application in the degradation of 1,4-dioxane using O3/UV/photocatalyst process. Separation and Purification Technology, 2020, 235, 116194.	3.9	23
1498	Mechanism of Î¼4-Opioid Receptor-Magnesium Interaction and Positive Allosteric Modulation. Biophysical Journal, 2020, 118, 909-921.	0.2	24
1499	Characteristics of a Folate Receptor-Î± Anchored into a Multilipid Bilayer Obtained from Atomistic Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 749-764.	2.3	5
1500	Properties of Aqueous Trehalose Mixtures: Glass Transition and Hydrogen Bonding. Journal of Chemical Theory and Computation, 2020, 16, 1249-1262.	2.3	39
1501	Voltage Sensing in Bacterial Protein Translocation. Biomolecules, 2020, 10, 78.	1.8	11
1502	Atomistic probing of aptameric binding of CD19 outer membrane domain reveals an â€œaptamer walkingâ€ mechanism. Biotechnology Progress, 2020, 36, e2957.	1.3	3
1503	Molecular Dynamics Study of the Human Beta-defensins 2 and 3 Chimeric Peptides with the Cell Membrane Model of Pseudomonas aeruginosa. International Journal of Peptide Research and Therapeutics, 2020, 26, 2039-2056.	0.9	5
1504	Exploring Ligand Stability in Protein Crystal Structures Using Binding Pose Metadynamics. Journal of Chemical Information and Modeling, 2020, 60, 1528-1539.	2.5	58
1505	Capturing Structural Transitions in Surfactant Adsorption Isotherms at Solid/Solution Interfaces. Langmuir, 2020, 36, 819-826.	1.6	4
1506	Enhanced wettability of long narrow carbon nanotubes in a double-walled hetero-structure: unraveling the effects of a boron nitride nanotube as the exterior. Physical Chemistry Chemical Physics, 2020, 22, 391-401.	1.3	6
1507	The regulation mechanism of phosphorylation and mutations in intrinsically disordered protein 4E-BP2. Physical Chemistry Chemical Physics, 2020, 22, 2938-2948.	1.3	5

#	ARTICLE	IF	CITATIONS
1508	Assessing the effect of aromatic residue placement on the α -helical peptide structure and nanofibril formation of 21-mer peptides. <i>Molecular Systems Design and Engineering</i> , 2020, 5, 521-531.	1.7	4
1509	Interaction of a Sarcolipin Pentamer and Monomer with the Sarcoplasmic Reticulum Calcium Pump, SERCA. <i>Biophysical Journal</i> , 2020, 118, 518-531.	0.2	13
1510	An in silico structural approach to characterize human and rainbow trout estrogenicity of mycotoxins: Proof of concept study using zearalenone and alternariol. <i>Food Chemistry</i> , 2020, 312, 126088.	4.2	20
1511	The Structural Basis for Low Conductance in the Membrane Protein VDAC upon β -NADH Binding and Voltage Gating. <i>Structure</i> , 2020, 28, 206-214.e4.	1.6	28
1512	Effect of Mixed-Solvent Environments on the Selectivity of Acid-Catalyzed Dehydration Reactions. <i>ACS Catalysis</i> , 2020, 10, 1679-1691.	5.5	45
1513	Microsecond-timescale simulations suggest 5-HT α 2-mediated preactivation of the 5-HT α 3 serotonin receptor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 405-414.	3.3	29
1514	A transglycosylating chitinase from <i>Chitiniphilus shinanonensis</i> (CsChIL) hydrolyzes chitin in a processive manner. <i>International Journal of Biological Macromolecules</i> , 2020, 145, 1-10.	3.6	17
1515	Catalytic Role of Gln202 in the Carbonylation Reaction Mechanism of Yeast AHAS: A QM/MM Study. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 915-922.	2.5	6
1516	ff19SB: Amino-Acid-Specific Protein Backbone Parameters Trained against Quantum Mechanics Energy Surfaces in Solution. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 528-552.	2.3	843
1517	A Minimal Membrane Metal Transport System: Dynamics and Energetics of <i>mer</i> Proteins. <i>Journal of Computational Chemistry</i> , 2020, 41, 528-537.	1.5	5
1518	Effect of cosolvents in the preferential binding affinity of water in aqueous solutions of amino acids and amides. <i>Journal of Molecular Liquids</i> , 2020, 300, 112375.	2.3	8
1519	The protein-water nuclear Overhauser effect (NOE) as an indirect microscope for molecular surface mapping of interaction patterns. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 212-222.	1.3	6
1520	Artificial water channels enable fast and selective water permeation through water-wire networks. <i>Nature Nanotechnology</i> , 2020, 15, 73-79.	15.6	111
1521	Exploring the role of elongation Factor-Like 1 (EFL1) in Shwachman-Diamond syndrome through molecular dynamics. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 5219-5229.	2.0	3
1522	BAND NN: A Deep Learning Framework for Energy Prediction and Geometry Optimization of Organic Small Molecules. <i>Journal of Computational Chemistry</i> , 2020, 41, 790-799.	1.5	26
1523	Ion Binding and Selectivity of the Na ⁺ /H ⁺ Antiporter MjNhaP1 from Experiment and Simulation. <i>Journal of Physical Chemistry B</i> , 2020, 124, 336-344.	1.2	8
1524	Role of the N-terminal Transmembrane Helix Contacts in the Activation of FGFR3. <i>Journal of Computational Chemistry</i> , 2020, 41, 561-572.	1.5	4
1525	Hierarchical Ensembles of Intrinsically Disordered Proteins at Atomic Resolution in Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 725-737.	2.3	63

#	ARTICLE	IF	CITATIONS
1526	Investigations of Albumin-Insulin Detemir Complexes Using Molecular Dynamics Simulations and Free Energy Calculations. <i>Molecular Pharmaceutics</i> , 2020, 17, 132-144.	2.3	8
1527	Exploring the role of the membrane bilayer in the recognition of candesartan by its GPCR AT1 receptor. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2020, 1862, 183142.	1.4	15
1528	Effect of Transmembrane Electric Field on GM1 Containing DMPC-Cholesterol Monolayer: A Computational Study. <i>Journal of Membrane Biology</i> , 2020, 253, 11-24.	1.0	1
1529	Do Molecular Dynamics Force Fields Capture Conformational Dynamics of Alanine in Water?. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 510-527.	2.3	22
1530	Top-down peeling bacterial cellulose to high strength ultrathin films and multifunctional fibers. <i>Chemical Engineering Journal</i> , 2020, 391, 123527.	6.6	33
1531	Interaction between mechanosensitive channels embedded in lipid membrane. <i>Journal of the Mechanical Behavior of Biomedical Materials</i> , 2020, 103, 103543.	1.5	2
1532	Implicit Micelle Model for Membrane Proteins Using Superellipsoid Approximation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 711-724.	2.3	10
1533	Membrane lipids are both the substrates and a mechanistically responsive environment of TMEM16 scramblase proteins. <i>Journal of Computational Chemistry</i> , 2020, 41, 538-551.	1.5	15
1534	Disentangling the role of solvent polarity and protein solvation in folding and self-assembly of β -lactalbumin. <i>Journal of Colloid and Interface Science</i> , 2020, 561, 749-761.	5.0	12
1535	Discovery of 5-aryl-3-thiophen-2-yl-1H-pyrazoles as a new class of Hsp90 inhibitors in hepatocellular carcinoma. <i>Bioorganic Chemistry</i> , 2020, 94, 103433.	2.0	8
1536	DHHC20 Palmitoyl-Transferase Reshapes the Membrane to Foster Catalysis. <i>Biophysical Journal</i> , 2020, 118, 980-988.	0.2	10
1537	Elucidation of interaction mechanism of hERG1 potassium channel with scorpion toxins BeKm-1 and BmTx3b. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 96, 107504.	1.3	3
1538	Prothrombin Arg541Trp Mutation Leads to Defective PC (Protein C) Pathway Activation and Constitutes a Novel Genetic Risk Factor for Venous Thrombosis. <i>Arteriosclerosis, Thrombosis, and Vascular Biology</i> , 2020, 40, 483-494.	1.1	8
1539	Identification of Zika Virus NS2B-NS3 Protease Inhibitors by Structure-Based Virtual Screening and Drug Repurposing Approaches. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 731-737.	2.5	36
1540	Mouse Models of Human Pathogenic Variants of TBC1D24 Associated with Non-Syndromic Deafness DFNB86 and DFNA65 and Syndromes Involving Deafness. <i>Genes</i> , 2020, 11, 1122.	1.0	12
1541	Unraveling the energetic significance of chemical events in enzyme catalysis via machine-learning based regression approach. <i>Communications Chemistry</i> , 2020, 3, .	2.0	16
1542	Molecular Modeling of Protein Kinases: Current Status and Challenges. <i>Topics in Medicinal Chemistry</i> , 2020, , 25-41.	0.4	0
1543	Characterization of the adipogenic protein E4orf1 from adenovirus 36 through an in silico approach. <i>Journal of Molecular Modeling</i> , 2020, 26, 285.	0.8	1

#	ARTICLE	IF	CITATIONS
1544	Computational Characterization of Antibody-Excipient Interactions for Rational Excipient Selection Using the Site Identification by Ligand Competitive Saturation-Biologics Approach. <i>Molecular Pharmaceutics</i> , 2020, 17, 4323-4333.	2.3	20
1545	Preventing the Interaction between Coronaviruses Spike Protein and Angiotensin I Converting Enzyme 2: An In Silico Mechanistic Case Study on Emodin as a Potential Model Compound. <i>Applied Sciences (Switzerland)</i> , 2020, 10, 6358.	1.3	4
1546	Characterization and engineering of a two-enzyme system for plastics depolymerization. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 25476-25485.	3.3	262
1547	Refining All-Atom Protein Force Fields for Polar-Rich, Prion-like, Low-Complexity Intrinsically Disordered Proteins. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9505-9512.	1.2	40
1548	Influences of electric fields on the operation of Aqp1 aquaporin channels: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25859-25868.	1.3	5
1549	Atomistic Structure and Dynamics of the Ca ²⁺ -ATPase Bound to Phosphorylated Phospholamban. <i>International Journal of Molecular Sciences</i> , 2020, 21, 7261.	1.8	6
1550	Structural and Computational Insights into a Blebbistatin-Bound Myosin-ADP Complex with Characteristics of an ADP-Release Conformation along the Two-Step Myosin Power Stroke. <i>International Journal of Molecular Sciences</i> , 2020, 21, 7417.	1.8	4
1551	Structural and Functional Insights into an Archaeal Lipid Synthase. <i>Cell Reports</i> , 2020, 33, 108294.	2.9	11
1552	Membrane surface recognition by the ASAP1 PH domain and consequences for interactions with the small GTPase Arf1. <i>Science Advances</i> , 2020, 6, .	4.7	26
1553	Formation of an unusual glutamine tautomer in a blue light using flavin photocycle characterizes the light-adapted state. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 26626-26632.	3.3	34
1554	Pulsed Electric Fields Can Create Pores in the Voltage Sensors of Voltage-Gated Ion Channels. <i>Biophysical Journal</i> , 2020, 119, 190-205.	0.2	43
1555	Barium blockade of the KcsA channel in open and closed conformation datasets. <i>Data in Brief</i> , 2020, 32, 106135.	0.5	1
1556	Thermal conductivity of the cell membrane in the presence of cholesterol and amyloid precursor protein. <i>Physical Review E</i> , 2020, 102, 042401.	0.8	3
1557	Distance-Dependent Cellular Uptake of Oligoproline-Based Homobivalent Ligands Targeting GPCRs—An Experimental and Computational Analysis. <i>Bioconjugate Chemistry</i> , 2020, 31, 2431-2438.	1.8	5
1558	Generalized correlation-based dynamical network analysis: a new high-performance approach for identifying allosteric communications in molecular dynamics trajectories. <i>Journal of Chemical Physics</i> , 2020, 153, 134104.	1.2	81
1559	In silico strategy for detailing the binding modes of a novel family of peptides proven as ghrelin receptor agonists. <i>Journal of Molecular Modeling</i> , 2020, 26, 294.	0.8	1
1560	Crystal structure of the periplasmic sensor domain of histidine kinase VbrK suggests indirect sensing of β -lactam antibiotics. <i>Journal of Structural Biology</i> , 2020, 212, 107610.	1.3	7
1561	The influence of polar and non-polar interactions on the self-assembly of peptide nanomembranes and their applications: An atomistic study using classical molecular dynamics. <i>Journal of Molecular Liquids</i> , 2020, 318, 114263.	2.3	15

#	ARTICLE	IF	CITATIONS
1562	Doxorubicin Stability and Retention on PEGylated Graphene Oxide Nanocarriers Adjacent to Human Serum Albumin. <i>ACS Applied Bio Materials</i> , 2020, 3, 7646-7653.	2.3	3
1563	Open and Closed Structures of a Barium-Blocked Potassium Channel. <i>Journal of Molecular Biology</i> , 2020, 432, 4783-4798.	2.0	14
1564	PLD2-PI(4,5)P2 interactions in fluid phase membranes: Structural modeling and molecular dynamics simulations. <i>PLoS ONE</i> , 2020, 15, e0236201.	1.1	5
1565	A Hybrid In Silico/In Vitro Target Fishing Study to Mine Novel Targets of Urolithin A and B: A Step Towards a Better Comprehension of Their Estrogenicity. <i>Molecular Nutrition and Food Research</i> , 2020, 64, e2000289.	1.5	10
1566	dUMP/F-dUMP Binding to Thymidylate Synthase: Human Versus <i>Mycobacterium tuberculosis</i> . <i>ACS Omega</i> , 2020, 5, 17182-17192.	1.6	1
1567	Transport Mechanism of Acetamide in Deep Eutectic Solvents. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1509-1520.	1.2	20
1568	Water Distribution and Clustering on the Lyophilized IgG1 Surface: Insight from Molecular Dynamics Simulations. <i>Molecular Pharmaceutics</i> , 2020, 17, 900-908.	2.3	6
1569	Next Generation Kinase Inhibitors. , 2020, , .		8
1570	Atomic-Level Characterization of the Methadone-Stabilized Active Conformation of μ -Opioid Receptor. <i>Molecular Pharmacology</i> , 2020, 98, 475-486.	1.0	16
1571	Molecular structure and interactions within amyloid-like fibrils formed by a low-complexity protein sequence from FUS. <i>Nature Communications</i> , 2020, 11, 5735.	5.8	76
1572	Lipid Dynamics in Membranes Slowed Down by Transmembrane Proteins. <i>Frontiers in Cell and Developmental Biology</i> , 2020, 8, 579388.	1.8	16
1573	Molecular dynamics simulation perception study of the binding affinity performance for main protease of SARS-CoV-2. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 2444-2459.	2.0	17
1574	Fast predictions of liquid-phase acid-catalyzed reaction rates using molecular dynamics simulations and convolutional neural networks. <i>Chemical Science</i> , 2020, 11, 12464-12476.	3.7	24
1575	Dividing the Periodic Box into Subdivisions with Their Surroundings to Accelerate Molecular Dynamics Simulation with High Accuracy. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7618-7631.	2.3	8
1576	The SERCA residue Glu340 mediates interdomain communication that guides Ca ²⁺ transport. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 31114-31122.	3.3	12
1577	Automated, Accurate, and Scalable Relative Protein-Ligand Binding Free-Energy Calculations Using Lambda Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7895-7914.	2.3	43
1578	Curli-Mediated Self-Assembly of a Fibrous Protein Scaffold for Hydroxyapatite Mineralization. <i>ACS Synthetic Biology</i> , 2020, 9, 3334-3343.	1.9	21
1579	A pleurocidin analogue with greater conformational flexibility, enhanced antimicrobial potency and in vivo therapeutic efficacy. <i>Communications Biology</i> , 2020, 3, 697.	2.0	14

#	ARTICLE	IF	CITATIONS
1580	1-(3-Tert-Butylphenyl)-2,2,2-Trifluoroethanone as a Potent Transition-State Analogue Slow-Binding Inhibitor of Human Acetylcholinesterase: Kinetic, MD and QM/MM Studies. <i>Biomolecules</i> , 2020, 10, 1608.	1.8	8
1581	Hydrogen-deuterium exchange mass spectrometry captures distinct dynamics upon substrate and inhibitor binding to a transporter. <i>Nature Communications</i> , 2020, 11, 6162.	5.8	35
1582	Multiscale Simulation Reveals Passive Proton Transport Through SERCA on the Microsecond Timescale. <i>Biophysical Journal</i> , 2020, 119, 1033-1040.	0.2	11
1583	Piecewise All-Atom SMD Simulations Reveal Key Secondary Structures in Luciferase Unfolding Pathway. <i>Biophysical Journal</i> , 2020, 119, 2251-2261.	0.2	3
1584	Toward Understanding CB[7]-Based Supramolecular Diels-Alder Catalysis. <i>Frontiers in Chemistry</i> , 2020, 8, 587084.	1.8	6
1585	Analyzing In Silico the Relationship Between the Activation of the Edema Factor and Its Interaction With Calmodulin. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 586544.	1.6	0
1586	Reversing the direction of drug transport mediated by the human multidrug transporter P-glycoprotein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 29609-29617.	3.3	28
1587	Different Force Fields Give Rise to Different Amyloid Aggregation Pathways in Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 6462-6475.	2.5	82
1588	Conformational changes in myeloperoxidase induced by ubiquitin and NETs containing free ISG15 from systemic lupus erythematosus patients promote a pro-inflammatory cytokine response in CD4+ T cells. <i>Journal of Translational Medicine</i> , 2020, 18, 429.	1.8	5
1589	Mutant thermal proteome profiling for characterization of missense protein variants and their associated phenotypes within the proteome. <i>Journal of Biological Chemistry</i> , 2020, 295, 16219-16238.	1.6	23
1590	Deep Learning in Protein Structural Modeling and Design. <i>Patterns</i> , 2020, 1, 100142.	3.1	119
1591	Nano-scale simulation of oil-water-nanosilica-rock system: Wettability and rheological properties alteration using charged nanoparticles. <i>Journal of Petroleum Science and Engineering</i> , 2020, 195, 107724.	2.1	4
1592	The Binding of Palonosetron and Other Antiemetic Drugs to the Serotonin 5-HT ₃ Receptor. <i>Structure</i> , 2020, 28, 1131-1140.e4.	1.6	20
1593	Design, Synthesis, and Biological Evaluation of Novel 7 <i>H</i> -[1,2,4]Triazolo[3,4- <i>b</i>][1,3,4]thiadiazine Inhibitors as Antitumor Agents. <i>ACS Omega</i> , 2020, 5, 20170-20186.	1.6	16
1594	Quantum Mechanics/Molecular Mechanics Study of Resting-State Vanadium Nitrogenase: Molecular and Electronic Structure of the Iron-Vanadium Cofactor. <i>Inorganic Chemistry</i> , 2020, 59, 11514-11527.	1.9	25
1595	Unifying the Contrasting Mechanisms of Protein-Stabilizing Osmolytes. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6565-6574.	1.2	26
1596	Dynamical properties of enzyme-substrate complexes disclose substrate specificity of the SARS-CoV-2 main protease as characterized by the electron density descriptors. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19069-19079.	1.3	29
1597	The Plasma Membrane as a Competitive Inhibitor and Positive Allosteric Modulator of KRas4B Signaling. <i>Biophysical Journal</i> , 2020, 118, 1129-1141.	0.2	40

#	ARTICLE	IF	CITATIONS
1598	Confinement in Nanodiscs Anisotropically Modifies Lipid Bilayer Elastic Properties. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7166-7175.	1.2	26
1599	Selection of mutant $\hat{\mu}$ plasmin for amyloid- $\hat{1}^2$ cleavage in vivo. <i>Scientific Reports</i> , 2020, 10, 12117.	1.6	4
1600	Characterizing the Hydration Properties of Proton Binding Sites in the ATP Synthase c-Rings of <i>Bacillus</i> Species. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7176-7183.	1.2	5
1601	Study on effects of co-solvents on the structure of DhaA by molecular dynamics simulation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 5999-6007.	2.0	0
1602	Molecular dynamics simulations provide molecular insights into the role of HLA-B*51 in Behçet's disease pathogenesis. <i>Chemical Biology and Drug Design</i> , 2020, 96, 644-658.	1.5	8
1603	Nucleotide-Specific Autoinhibition of Full-Length K-Ras4B Identified by Extensive Conformational Sampling. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 145.	1.6	11
1604	Structure-guided evolution of Green2 toward photostability and quantum yield enhancement by F145Y substitution. <i>Protein Science</i> , 2020, 29, 1964-1974.	3.1	2
1605	Aggregation of 25-hydroxycholesterol in a complex biomembrane. Differences with cholesterol. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2020, 1862, 183413.	1.4	12
1606	Can CHARMM36 atomic charges described correctly the interaction between amino acid and water molecules by molecular dynamics simulations?. <i>Journal of Molecular Liquids</i> , 2020, 317, 113919.	2.3	18
1607	Determinants of Endoplasmic Reticulum-to-Lipid Droplet Protein Targeting. <i>Developmental Cell</i> , 2020, 54, 471-487.e7.	3.1	42
1608	The Human TSH $\hat{2}$ Subunit Proteins and Their Binding Sites on the TSH Receptor Using Molecular Dynamics Simulation. <i>Endocrinology</i> , 2020, 161, .	1.4	1
1609	Permutationally Invariant, Reproducing Kernel-Based Potential Energy Surfaces for Polyatomic Molecules: From Formaldehyde to Acetone. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5474-5484.	2.3	37
1610	Bifurcated Hydrogen Bonds and the Fold Switching of Lymphotoctin. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6555-6564.	1.2	7
1611	Identification of an $\hat{1}^{\pm}$ -MoRF in the Intrinsically Disordered Region of the Escargot Transcription Factor. <i>ACS Omega</i> , 2020, 5, 18331-18341.	1.6	0
1612	Infinite switch simulated tempering in force (FISST). <i>Journal of Chemical Physics</i> , 2020, 152, 244120.	1.2	12
1613	Exploration of Alternative Scaffolds for P2Y ₁₄ Receptor Antagonists Containing a Biaryl Core. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 9563-9589.	2.9	20
1614	Structural Characterization of <i>Sphingomonas</i> sp. KT-1 PahZ1-Catalyzed Biodegradation of Thermally Synthesized Poly(aspartic acid). <i>ACS Sustainable Chemistry and Engineering</i> , 2020, , .	3.2	1
1615	CHARMM-GUI supports the Amber force fields. <i>Journal of Chemical Physics</i> , 2020, 153, 035103.	1.2	175

#	ARTICLE	IF	CITATIONS
1616	The Droserasin 1 PSI: A Membrane-Interacting Antimicrobial Peptide from the Carnivorous Plant <i>Drosera capensis</i> . <i>Biomolecules</i> , 2020, 10, 1069.	1.8	7
1617	A6H polypeptide membranes: Molecular dynamics simulation, GIAO-DFT-NMR and TD-DFT spectroscopy analysis. <i>Journal of Molecular Liquids</i> , 2020, 316, 113850.	2.3	19
1618	On the Functional Annotation of Open-Channel Structures in the Glycine Receptor. <i>Structure</i> , 2020, 28, 690-693.e3.	1.6	9
1619	An embedded lipid in the multidrug transporter LmrP suggests a mechanism for polyspecificity. <i>Nature Structural and Molecular Biology</i> , 2020, 27, 829-835.	3.6	57
1620	Potential toxicity mechanism of MoS2 nanotube in the interaction between YAP65 WW domain and PRM. <i>Colloids and Surfaces B: Biointerfaces</i> , 2020, 196, 111317.	2.5	2
1621	A machine learning study of the two states model for lipid bilayer phase transitions. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19147-19154.	1.3	11
1622	Removal of N-linked glycans in cellobiohydrolase Cel7A from <i>Trichoderma reesei</i> reveals higher activity and binding affinity on crystalline cellulose. <i>Biotechnology for Biofuels</i> , 2020, 13, 136.	6.2	15
1623	Investigating the Role of the N-Terminal Loop of PD-1 in Binding Process Between PD-1 and Nivolumab via Molecular Dynamics Simulation. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 574759.	1.6	6
1624	Accurate modeling of a biological nanopore with an extended continuum framework. <i>Nanoscale</i> , 2020, 12, 16775-16795.	2.8	26
1625	MARTINI-Compatible Coarse-Grained Model for the Mesoscale Simulation of Peptoids. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7745-7764.	1.2	28
1626	Effect of surface structure on peptide adsorption on soft surfaces. <i>Chemical Physics Letters</i> , 2020, 758, 137929.	1.2	2
1627	MDBenchmark: A toolkit to optimize the performance of molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2020, 153, 144105.	1.2	10
1628	On the faithfulness of molecular mechanics representations of proteins towards quantum-mechanical energy surfaces. <i>Interface Focus</i> , 2020, 10, 20190121.	1.5	13
1629	The structure of the antimicrobial human cathelicidin LL-37 shows oligomerization and channel formation in the presence of membrane mimics. <i>Scientific Reports</i> , 2020, 10, 17356.	1.6	54
1630	CHARMM-GUI Free Energy Calculator for Absolute and Relative Ligand Solvation and Binding Free Energy Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7207-7218.	2.3	57
1631	Critical Sequence Hotspots for Binding of Novel Coronavirus to Angiotensin Converter Enzyme as Evaluated by Molecular Simulations. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10034-10047.	1.2	54
1632	High-throughput virtual screening of drug databanks for potential inhibitors of SARS-CoV-2 spike glycoprotein. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 2099-2112.	2.0	28
1633	Using Simulation to Understand the Role of Titration on the Stability of a Peptide-Lipid Bilayer Complex. <i>Langmuir</i> , 2020, 36, 12272-12280.	1.6	3

#	ARTICLE	IF	CITATIONS
1634	A restrained locally enhanced sampling method (RLES) for finding free energy minima in complex systems. <i>Journal of Chemical Physics</i> , 2020, 153, 121103.	1.2	1
1635	Deciphering collaborative sidechain motions in proteins during molecular dynamics simulations. <i>Scientific Reports</i> , 2020, 10, 15901.	1.6	7
1636	Polyol and sugar osmolytes can shorten protein hydrogen bonds to modulate function. <i>Communications Biology</i> , 2020, 3, 528.	2.0	20
1637	Biomedical Science to Tackle the COVID-19 Pandemic: Current Status and Future Perspectives. <i>Molecules</i> , 2020, 25, 4620.	1.7	23
1638	In silico analysis of the strigolactone ligand-receptor system. <i>Plant Direct</i> , 2020, 4, e00263.	0.8	8
1639	Rapid Formation of Peptide/Lipid Coaggregates by the Amyloidogenic Seminal Peptide PAP248-286. <i>Biophysical Journal</i> , 2020, 119, 924-938.	0.2	6
1640	Interaction Mechanism of the Germination Stimulants Karrikins and Their Receptor ShKAI2iB. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9812-9819.	1.2	8
1641	Molecular level investigation of curcumin self-assembly induced by trigonelline and nanoparticle formation. <i>Applied Nanoscience (Switzerland)</i> , 2020, 10, 3987-3998.	1.6	4
1642	Shared structural mechanisms of general anaesthetics and benzodiazepines. <i>Nature</i> , 2020, 585, 303-308.	13.7	195
1643	Molecular mechanism of mitochondrial phosphatidate transfer by Ups1. <i>Communications Biology</i> , 2020, 3, 468.	2.0	6
1644	An Unusual Amino Acid Substitution Within Hummingbird Cytochrome <i>c</i> Oxidase Alters a Key Proton-Conducting Channel. <i>G3: Genes, Genomes, Genetics</i> , 2020, 10, 2477-2485.	0.8	4
1645	Roles of variable linker length in dual acting virucidal entry inhibitors on HIV-1 potency via on-the-fly free energy molecular simulations. <i>Protein Science</i> , 2020, 29, 2304-2310.	3.1	3
1646	Assessing the Perturbing Effects of Drugs on Lipid Bilayers Using Gramicidin Channel-Based <i>In Silico</i> and <i>In Vitro</i> Assays. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 11809-11818.	2.9	10
1647	Cholesterol Localization around the Metabotropic Glutamate Receptor 2. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9061-9078.	1.2	3
1648	A Novel Cytotoxic Conjugate Derived from the Natural Product Podophyllotoxin as a Direct-Target Protein Dual Inhibitor. <i>Molecules</i> , 2020, 25, 4258.	1.7	7
1649	Several coumarin derivatives and their Pd(II) complexes as potential inhibitors of the main protease of SARS-CoV-2, an <i>in silico</i> approach. <i>RSC Advances</i> , 2020, 10, 35099-35108.	1.7	37
1650	Theoretical Study of Intermolecular Interactions between Critical Residues of Membrane Protein MrAY _{AA} and Promising Antibiotic Muraymycin D2. <i>ACS Omega</i> , 2020, 5, 22739-22749.	1.6	5
1651	Structure and Function of the T4 Spackle Protein Gp61.3. <i>Viruses</i> , 2020, 12, 1070.	1.5	4

#	ARTICLE	IF	CITATIONS
1652	The Effects of <i>p</i> -Azidophenylalanine Incorporation on Protein Structure and Stability. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5117-5125.	2.5	6
1653	Role of alkylated residues in the tetrapeptide self-assembly: A molecular dynamics study. <i>Journal of Computational Chemistry</i> , 2020, 41, 2634-2640.	1.5	2
1654	Unraveling the complex enzymatic machinery making a key galactolipid in chloroplast membrane: a multiscale computer simulation. <i>Scientific Reports</i> , 2020, 10, 13514.	1.6	10
1655	Bedaquiline inhibits the yeast and human mitochondrial ATP synthases. <i>Communications Biology</i> , 2020, 3, 452.	2.0	32
1656	Solvation and transport of lithium ions in deep eutectic solvents. <i>Journal of Chemical Physics</i> , 2020, 153, 104505.	1.2	17
1657	Discovery of potent inhibitors for SARS-CoV-2's main protease by ligand-based/structure-based virtual screening, MD simulations, and binding energy calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 23099-23106.	1.3	29
1658	Assessment of Force Field Accuracy Using Cryogenic Electron Microscopy Data of Hyper-thermostable Glutamate Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2020, 124, 8479-8494.	1.2	2
1659	Glycine in Water Favors the Polyproline II State. <i>Biomolecules</i> , 2020, 10, 1121.	1.8	15
1660	Protein Surface Printer for Exploring Protein Domains. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5255-5264.	2.5	2
1661	Structural cavities are critical to balancing stability and activity of a membrane-integral enzyme. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 22146-22156.	3.3	23
1662	High force catch bond mechanism of bacterial adhesion in the human gut. <i>Nature Communications</i> , 2020, 11, 4321.	5.8	40
1663	Sequence Characterization and Molecular Modeling of Clinically Relevant Variants of the SARS-CoV-2 Main Protease. <i>Biochemistry</i> , 2020, 59, 3741-3756.	1.2	30
1664	The solution structure of the complement deregulator FHR5 reveals a compact dimer and provides new insights into CFHR5 nephropathy. <i>Journal of Biological Chemistry</i> , 2020, 295, 16342-16358.	1.6	3
1665	Molecular computations of preferential interactions of proline, arginine.HCl, and NaCl with IgG1 antibodies and their impact on aggregation and viscosity. <i>MAbs</i> , 2020, 12, 1816312.	2.6	17
1666	A molecular dynamic simulation approach: development of dengue virus vaccine by affinity improvement techniques. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 61-76.	2.0	3
1667	Systematic Parameterization and Simulation of Boronic Acid ²⁻ -Lactamase Aqueous Solution in Developing the ABEEM ²⁻ Polarizable Force Field. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8614-8632.	1.1	8
1668	Repurposing of FDA-Approved Toremifene to Treat COVID-19 by Blocking the Spike Glycoprotein and NSP14 of SARS-CoV-2. <i>Journal of Proteome Research</i> , 2020, 19, 4670-4677.	1.8	55
1669	Enhancing cellulosic ethanol production through coevolution of multiple enzymatic characteristics of β -glucosidase from <i>Penicillium oxalicum</i> 16. <i>Applied Microbiology and Biotechnology</i> , 2020, 104, 8299-8308.	1.7	10

#	ARTICLE	IF	CITATIONS
1670	ADD Force Field for Sugars and Polyols: Predicting the Additivity of Protein-Osmolyte Interaction. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7779-7790.	1.2	11
1671	Machine Learning Models of Antibody-Excipient Preferential Interactions for Use in Computational Formulation Design. <i>Molecular Pharmaceutics</i> , 2020, 17, 3589-3599.	2.3	17
1672	Multi-level free energy simulation with a staged transformation approach. <i>Journal of Chemical Physics</i> , 2020, 153, 044115.	1.2	13
1673	A computational structural study on the DNA-protecting role of the tardigrade-unique Dsup protein. <i>Scientific Reports</i> , 2020, 10, 13424.	1.6	25
1674	Conformational transition of SARS-CoV-2 spike glycoprotein between its closed and open states. <i>Journal of Chemical Physics</i> , 2020, 153, 075101.	1.2	111
1675	Parameters for Irreversible Inactivation of Monoamine Oxidase. <i>Molecules</i> , 2020, 25, 5908.	1.7	10
1676	Impact of Sucrose as Osmolyte on Molecular Dynamics of Mouse Acetylcholinesterase. <i>Biomolecules</i> , 2020, 10, 1664.	1.8	10
1677	CGMD Platform: Integrated Web Servers for the Preparation, Running, and Analysis of Coarse-Grained Molecular Dynamics Simulations. <i>Molecules</i> , 2020, 25, 5934.	1.7	14
1678	Influence of Different Aromatic Hydrophobic Residues on the Antimicrobial Activity and Membrane Selectivity of BRBR-NH ₂ Tetrapeptide. <i>Langmuir</i> , 2020, 36, 15331-15342.	1.6	6
1679	Extended H-Bonding through Protic Ionic Liquids Facilitates the Growth and Stability of Water Domains in Hydrophobic Environment. <i>Langmuir</i> , 2020, 36, 15362-15372.	1.6	3
1680	Non-canonical Shedding of TNF α by SPPL2a Is Determined by the Conformational Flexibility of Its Transmembrane Helix. <i>IScience</i> , 2020, 23, 101775.	1.9	14
1681	Quantification of the Resilience and Vulnerability of HIV-1 Native Glycan Shield at Atomistic Detail. <i>IScience</i> , 2020, 23, 101836.	1.9	11
1682	Functional Water Wires Catalyze Long-Range Proton Pumping in the Mammalian Respiratory Complex I. <i>Journal of the American Chemical Society</i> , 2020, 142, 21758-21766.	6.6	25
1683	Simulating selective binding of a biological template to a nanoscale architecture: a core concept of a clamp-based binding-pocket-favored N-terminal-domain assembly. <i>Nanoscale</i> , 2020, 12, 24214-24227.	2.8	18
1684	How GPCR Phosphorylation Patterns Orchestrate Arrestin-Mediated Signaling. <i>Cell</i> , 2020, 183, 1813-1825.e18.	13.5	100
1685	Quantitative study of unsaturated transport of glycerol through aquaglyceroporin that has high affinity for glycerol. <i>RSC Advances</i> , 2020, 10, 34203-34214.	1.7	4
1686	Structural insights into the mechanism of rhodopsin phosphodiesterase. <i>Nature Communications</i> , 2020, 11, 5605.	5.8	30
1687	Multi-epitope vaccine against SARS-CoV-2 applying immunoinformatics and molecular dynamics simulation approaches. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 2917-2933.	2.0	26

#	ARTICLE	IF	CITATIONS
1688	Examination of the Role of Mg ²⁺ in the Mechanism of Nucleotide Binding to the Monomeric YME1L AAA+ Domain. <i>Biochemistry</i> , 2020, 59, 4303-4320.	1.2	3
1689	Impact of Cholesterol Concentration and Lipid Phase on Structure and Fluctuation of Amyloid Precursor Protein. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10173-10185.	1.2	9
1690	Neutral Peptides in the Gas Phase: Conformation and Aggregation Issues. <i>Chemical Reviews</i> , 2020, 120, 12490-12562.	23.0	40
1691	Shifting Polar Residues Across Primary Sequence Frames of Transmembrane Domains Calibrates Membrane Permeation Thermodynamics. <i>Biochemistry</i> , 2020, 59, 4353-4366.	1.2	0
1692	Structural basis for divergent and convergent evolution of catalytic machineries in plant aromatic amino acid decarboxylase proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 10806-10817.	3.3	34
1693	Molecular Simulation of \hat{v}^26 Integrin Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5487-5498.	2.5	7
1694	Behavior of anchor functionalized ZnPc molecules on a graphene nanoflake near membrane cell. <i>Structural Chemistry</i> , 2020, 31, 1935-1943.	1.0	1
1695	Semiclassical Vibrational Spectroscopy of Biological Molecules Using Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3476-3485.	2.3	18
1696	Identification of the New Covalent Allosteric Binding Site of Fructose-1,6-bisphosphatase with Disulfiram Derivatives toward Glucose Reduction. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 6238-6247.	2.9	17
1697	Structural and functional insights into oligopeptide acquisition by the RagAB transporter from <i>Porphyromonas gingivalis</i> . <i>Nature Microbiology</i> , 2020, 5, 1016-1025.	5.9	46
1698	Structural analyses and force fields comparison for NACore (68â€“78) and SubNACore (69â€“77) fibril segments of Parkinsonâ€™s disease. <i>Journal of Molecular Modeling</i> , 2020, 26, 132.	0.8	3
1699	Insights into the Sensitivity of Arginine Concentration to Preserve the Folded Form of Insulin Monomer under Thermal Stress. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3105-3119.	2.5	9
1700	A structurally minimized yet fully active insulin based on cone-snail venom insulin principles. <i>Nature Structural and Molecular Biology</i> , 2020, 27, 615-624.	3.6	36
1701	Computational Modeling of Ion Transport in Bulk and through a Nanopore Using the Drude Polarizable Force Field. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3188-3203.	2.5	16
1702	Application of the Brown Dynamics Fluctuation-Dissipation Theorem to the Study of Plasmodium berghei Transporter Protein PbAQP. <i>Frontiers in Physics</i> , 2020, 8, .	1.0	0
1703	Targeting Intrinsically Disordered Proteins through Dynamic Interactions. <i>Biomolecules</i> , 2020, 10, 743.	1.8	34
1704	Structural Similarity with Cholesterol Reveals Crucial Insights into Mechanisms Sustaining the Immunomodulatory Activity of the Mycotoxin Alternariol. <i>Cells</i> , 2020, 9, 847.	1.8	20
1705	Cu(I) Controls Conformational States in Human Atox1 Metallochaperone: An EPR and Multiscale Simulation Study. <i>Journal of Physical Chemistry B</i> , 2020, 124, 4399-4411.	1.2	10

#	ARTICLE	IF	CITATIONS
1706	Long-range Regulation of Partially Folded Amyloidogenic Peptides. <i>Scientific Reports</i> , 2020, 10, 7597.	1.6	12
1707	A role for actin flexibility in thin filament-mediated contractile regulation and myopathy. <i>Nature Communications</i> , 2020, 11, 2417.	5.8	16
1708	Mesoscale computational protocols for the design of highly cooperative bivalent macromolecules. <i>Scientific Reports</i> , 2020, 10, 7992.	1.6	0
1709	Biophysical and computational view on the <i>in vitro</i> combination between an anticancer drug, saracatinib and human serum albumin. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 3565-3575.	2.0	7
1710	In silico identification of new inhibitors for Î²eta-2-glycoprotein I as a major antigen in antiphospholipid antibody syndrome. <i>Journal of Molecular Modeling</i> , 2020, 26, 156.	0.8	6
1711	Theoretical study of ciprofloxacin antibiotic trapping on graphene or boron nitride oxide nanoflakes. <i>Journal of Molecular Modeling</i> , 2020, 26, 135.	0.8	12
1712	Loss of m1acp3 ⁺ Ribosomal RNA Modification Is a Major Feature of Cancer. <i>Cell Reports</i> , 2020, 31, 107611.	2.9	64
1713	Comparison of Reaction Field Schemes for Coupling Continuum Solvation Models with Wave Function Methods for Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4554-4564.	2.3	7
1714	Electromechanical coupling in the hyperpolarization-activated K ⁺ channel KAT1. <i>Nature</i> , 2020, 583, 145-149.	13.7	51
1715	Structural Analysis of an <i>scp</i> -Cysteine Desulfurase from an Ssp DNA Phosphorothioation System. <i>MBio</i> , 2020, 11, .	1.8	8
1716	pKa Calculations with the Polarizable Drude Force Field and Poisson-Boltzmann Solvation Model. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4655-4668.	2.3	14
1717	Tracking Ca ²⁺ ATPase intermediates in real time by x-ray solution scattering. <i>Science Advances</i> , 2020, 6, eaaz0981.	4.7	29
1718	PKA and Ube3a regulate SK2 channel trafficking to promote synaptic plasticity in hippocampus: Implications for Angelman Syndrome. <i>Scientific Reports</i> , 2020, 10, 9824.	1.6	7
1719	Human aminolevulinatase synthase structure reveals a eukaryotic-specific autoinhibitory loop regulating substrate binding and product release. <i>Nature Communications</i> , 2020, 11, 2813.	5.8	25
1720	<i>In silico</i> simulations of erythrocyte aquaporins with quantitative <i>in vitro</i> validation. <i>RSC Advances</i> , 2020, 10, 21283-21291.	1.7	6
1721	Atomistic mechanism of transmembrane helix association. <i>PLoS Computational Biology</i> , 2020, 16, e1007919.	1.5	16
1722	Enhanced receptor binding of SARS-CoV-2 through networks of hydrogen-bonding and hydrophobic interactions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 13967-13974.	3.3	291
1723	Toward empirical force fields that match experimental observables. <i>Journal of Chemical Physics</i> , 2020, 152, 230902.	1.2	49

#	ARTICLE	IF	CITATIONS
1724	Conformational Free-Energy Differences of Large Solvated Systems with the Focused Confinement Method. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5163-5173.	2.3	4
1725	Developing a Fully Glycosylated Full-Length SARS-CoV-2 Spike Protein Model in a Viral Membrane. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7128-7137.	1.2	240
1726	Cell Membrane Penetration without Pore Formation: Chameleonic Properties of Dendrimers in Response to Hydrophobic and Hydrophilic Environments. <i>Advanced Theory and Simulations</i> , 2020, 3, 1900152.	1.3	2
1727	Unfolding Dynamics of a Photoswitchable Helical Peptide. <i>Journal of Physical Chemistry B</i> , 2020, 124, 5380-5392.	1.2	3
1728	Insulin Dissociates by Diverse Mechanisms of Coupled Unfolding and Unbinding. <i>Journal of Physical Chemistry B</i> , 2020, 124, 5571-5587.	1.2	35
1729	Thermodynamic Integration in 3n Dimensions Without Biases or Alchemy for Protein Interactions. <i>Frontiers in Physics</i> , 2020, 8, .	1.0	0
1730	Hydrogen bond network analysis reveals the pathway for the proton transfer in the E-channel of T. thermophilus Complex I. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2020, 1861, 148240.	0.5	20
1731	Hydrogen bonds and hydrate interaction between RiAFP and water revealed by molecular dynamics simulations. <i>Chemical Physics</i> , 2020, 538, 110860.	0.9	3
1732	Three Popular Force Fields Predict Consensus Mechanism of Amyloid β Peptide Binding to the Dimyristoylglycerophosphocholine Bilayer. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2282-2293.	2.5	11
1733	Identifying mutation hotspots reveals pathogenetic mechanisms of KCNQ2 epileptic encephalopathy. <i>Scientific Reports</i> , 2020, 10, 4756.	1.6	42
1734	Sonification based <i>de novo</i> protein design using artificial intelligence, structure prediction, and analysis using molecular modeling. <i>APL Bioengineering</i> , 2020, 4, 016108.	3.3	36
1735	Spontaneous Hinge-Bending Motions of Angiotensin I Converting Enzyme: Role in Activation and Inhibition. <i>Molecules</i> , 2020, 25, 1288.	1.7	9
1736	Structural Investigation of the Vitamin K Epoxide Reductase (VKORC1) Binding Site with Vitamin K. <i>Biochemistry</i> , 2020, 59, 1351-1360.	1.2	6
1737	pH-Induced Changes in Polypeptide Conformation: Force-Field Comparison with Experimental Validation. <i>Journal of Physical Chemistry B</i> , 2020, 124, 2961-2972.	1.2	29
1738	Chiral twisting in a bacterial cytoskeletal polymer affects filament size and orientation. <i>Nature Communications</i> , 2020, 11, 1408.	5.8	24
1739	Conformational dynamics modulate the catalytic activity of the molecular chaperone Hsp90. <i>Nature Communications</i> , 2020, 11, 1410.	5.8	50
1740	A hallmark of phospholamban functional divergence is located in the N-terminal phosphorylation domain. <i>Computational and Structural Biotechnology Journal</i> , 2020, 18, 705-713.	1.9	3
1741	Verification of sortase for protein conjugation by single-molecule force spectroscopy and molecular dynamics simulations. <i>Chemical Communications</i> , 2020, 56, 3943-3946.	2.2	22

#	ARTICLE	IF	CITATIONS
1742	Conformational spread and dynamics in allostery of NMDA receptors. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 3839-3847.	3.3	25
1743	Mapping of Ion and Substrate Binding Sites in Human Sodium Iodide Symporter (hNIS). Journal of Chemical Information and Modeling, 2020, 60, 1652-1665.	2.5	8
1744	Register-shift-insulin analogs uncover constraints of proteotoxicity in protein evolution. Journal of Biological Chemistry, 2020, 295, 3080-3098.	1.6	11
1745	Efficient Estimation of Absolute Binding Free Energy for a Homeodomain-DNA Complex from Nonequilibrium Pulling Simulations. Journal of Chemical Theory and Computation, 2020, 16, 2034-2041.	2.3	7
1746	Cinnamoyl-coumarin hybrid derivatives with remarkable fluorescent molecular-rotor properties in mixtures of DPPC:DOPC LUVs. Dyes and Pigments, 2020, 178, 108356.	2.0	5
1747	Ten quick tips for homology modeling of high-resolution protein 3D structures. PLoS Computational Biology, 2020, 16, e1007449.	1.5	75
1748	Assessment of the Multifunctional Behavior of Lupin Peptide P7 and Its Metabolite Using an Integrated Strategy. Journal of Agricultural and Food Chemistry, 2020, 68, 13179-13188.	2.4	24
1749	In silico design and validation of high-affinity RNA aptamers targeting epithelial cellular adhesion molecule dimers. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 8486-8493.	3.3	49
1750	Development and Characterization of the Shortest Anti-Adhesion Peptide Analogue of B49Mod1. Molecules, 2020, 25, 1188.	1.7	5
1751	Membrane Phospholipid Analogues as Molecular Rulers to Probe the Position of the Hydrophobic Contact Point of Lysophospholipid Ligands on the Surface of G-Protein-Coupled Receptor during Membrane Approach. Biochemistry, 2020, 59, 1173-1201.	1.2	4
1752	Impact of Thiol-Disulfide Balance on the Binding of Covid-19 Spike Protein with Angiotensin-Converting Enzyme 2 Receptor. ACS Omega, 2020, 5, 16292-16298.	1.6	140
1753	The mechanism and energetics of a ligand-controlled hydrophobic gate in a mammalian two pore channel. Physical Chemistry Chemical Physics, 2020, 22, 15664-15674.	1.3	13
1754	New Molecular-Mechanics Model for Simulations of Hydrogen Fluoride in Chemistry and Biology. Journal of Chemical Theory and Computation, 2020, 16, 5105-5126.	2.3	15
1755	Structure of the Brain <i>N</i> -Acetylaspartate Biosynthetic Enzyme NAT8L Revealed by Computer Modeling. ACS Chemical Neuroscience, 2020, 11, 2296-2302.	1.7	4
1756	Update of the CHARMM36 United Atom Chain Model for Hydrocarbons and Phospholipids. Journal of Physical Chemistry B, 2020, 124, 6797-6812.	1.2	16
1757	Using the generalized Born surface area model to fold proteins yields more effective sampling while qualitatively preserving the folding landscape. Physical Review E, 2020, 101, 062417.	0.8	5
1758	Co-evolution of Î²-glucosidase activity and product tolerance for increasing cellulosic ethanol yield. Biotechnology Letters, 2020, 42, 2239-2250.	1.1	8
1759	Water Dynamics Around Proteins: T- and R-States of Hemoglobin and Melittin. Journal of Physical Chemistry B, 2020, 124, 6540-6554.	1.2	16

#	ARTICLE	IF	CITATIONS
1760	Acquired Functional Capsid Structures in Metazoan Totivirus-like dsRNA Virus. <i>Structure</i> , 2020, 28, 888-896.e3.	1.6	12
1761	Anionic Lipids Impact RAS-Binding Site Accessibility and Membrane Binding Affinity of CRAF RBD-CRD. <i>Biophysical Journal</i> , 2020, 119, 525-538.	0.2	13
1762	Assessing the DOPC-cholesterol interactions and their influence on fullerene C60 partitioning in lipid bilayers. <i>Journal of Molecular Liquids</i> , 2020, 315, 113698.	2.3	15
1763	EPR Distance Measurements on Long Non-coding RNAs Empowered by Genetic Alphabet Expansion Transcription. <i>Angewandte Chemie</i> , 2020, 132, 7965-7970.	1.6	9
1764	Biophysical and in silico investigations of the molecular association between a potent RNA polymerase inhibitor, thiolutin and human serum albumin. <i>Journal of Molecular Liquids</i> , 2020, 303, 112648.	2.3	10
1765	Predicting NMR relaxation of proteins from molecular dynamics simulations with accurate methyl rotation barriers. <i>Journal of Chemical Physics</i> , 2020, 152, 084102.	1.2	22
1766	Donepezil Inhibits Acetylcholinesterase via Multiple Binding Modes at Room Temperature. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3463-3471.	2.5	35
1767	Proof of concept for poor inhibitor binding and efficient formation of covalent adducts of KRAS ^{G12C} and ARS compounds. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 3069-3081.	1.5	16
1768	Optimization of a Benzothiazole Indolene Scaffold Targeting Bacterial Cell Wall Assembly. <i>Drug Design, Development and Therapy</i> , 2020, Volume 14, 567-574.	2.0	5
1769	Single-channel properties of skeletal muscle ryanodine receptor pore γ 4923FF4924 in two brothers with a lethal form of fetal akinesia. <i>Cell Calcium</i> , 2020, 87, 102182.	1.1	6
1770	Interactions between trans-resveratrol and CpLIP2 lipase/acyltransferase: Evidenced by fluorescence and in silico. <i>Food Chemistry</i> , 2020, 318, 126482.	4.2	13
1771	The hydrolysis mechanism of a GH45 cellulase and its potential relation to lytic transglycosylase and expansin function. <i>Journal of Biological Chemistry</i> , 2020, 295, 4477-4487.	1.6	16
1772	C-terminal residues of activated protein C light chain contribute to its anticoagulant and cytoprotective activities. <i>Journal of Thrombosis and Haemostasis</i> , 2020, 18, 1027-1038.	1.9	4
1773	Modulation of Toroidal Proteins Dynamics in Favor of Functional Mechanisms upon Ligand Binding. <i>Biophysical Journal</i> , 2020, 118, 1782-1794.	0.2	9
1774	The Ca ²⁺ permeation mechanism of the ryanodine receptor revealed by a multi-site ion model. <i>Nature Communications</i> , 2020, 11, 922.	5.8	33
1775	Molecular mechanism of biased signaling in a prototypical G protein-coupled receptor. <i>Science</i> , 2020, 367, 881-887.	6.0	168
1776	Trinuclear copper biocatalytic center forms an active site of thiocyanate dehydrogenase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 5280-5290.	3.3	19
1777	The Arabidopsis (ASHH2) CW domain binds monomethylated K4 of the histone H3 tail through conformational selection. <i>FEBS Journal</i> , 2020, 287, 4458-4480.	2.2	4

#	ARTICLE	IF	CITATIONS
1778	BamA is required for autotransporter secretion. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2020, 1864, 129581.	1.1	10
1779	CL-FEP: An End-State Free Energy Perturbation Approach. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1396-1410.	2.3	8
1780	Microsecond Molecular Dynamics Simulations of Proteins Using a Quasi-Equilibrium Solvation Shell Model. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1866-1881.	2.3	9
1781	A Conserved Kinase-Based Body-Temperature Sensor Globally Controls Alternative Splicing and Gene Expression. <i>Molecular Cell</i> , 2020, 78, 57-69.e4.	4.5	76
1782	Outer membrane protein size and LPS O-antigen define protective antibody targeting to the Salmonella surface. <i>Nature Communications</i> , 2020, 11, 851.	5.8	49
1783	Molecular Insights into the Loading and Dynamics of Doxorubicin on PEGylated Graphene Oxide Nanocarriers. <i>ACS Applied Bio Materials</i> , 2020, 3, 1354-1363.	2.3	37
1784	Rationally designed antimicrobial peptides: Insight into the mechanism of eleven residue peptides against microbial infections. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2020, 1862, 183177.	1.4	21
1785	Location, Orientation and Aggregation of Bardoxolone-ME, CDDO-ME, in a Complex Phospholipid Bilayer Membrane. <i>Journal of Membrane Biology</i> , 2020, 253, 115-128.	1.0	2
1786	A spontaneous mitonuclear epistasis converging on Rieske Fe-S protein exacerbates complex III deficiency in mice. <i>Nature Communications</i> , 2020, 11, 322.	5.8	17
1787	Structural Characterization of the CD44 Stem Region for Standard and Cancer-Associated Isoforms. <i>International Journal of Molecular Sciences</i> , 2020, 21, 336.	1.8	9
1788	Potential of Matrix Metalloproteinase Inhibitors for the Treatment of Local Tissue Damage Induced by a Type P-I Snake Venom Metalloproteinase. <i>Toxins</i> , 2020, 12, 8.	1.5	7
1789	Structural instability and divergence from conserved residues underlie intracellular retention of mammalian odorant receptors. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 2957-2967.	3.3	27
1790	Scorpion toxin inhibits the voltage-gated proton channel using a Zn ²⁺ -like long-range conformational coupling mechanism. <i>British Journal of Pharmacology</i> , 2020, 177, 2351-2364.	2.7	14
1791	EPR Distance Measurements on Long Non-coding RNAs Empowered by Genetic Alphabet Expansion Transcription. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 7891-7896.	7.2	30
1792	Molecular Insight into the Interaction between Camptothecin and Acyclic Cucurbit[4]urils as Efficient Nanocontainers in Comparison with Cucurbit[7]uril: Molecular Docking and Molecular Dynamics Simulation. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1791-1803.	2.5	10
1793	Mechanical Unfolding of Spectrin Repeats Induces Water-Molecule Ordering. <i>Biophysical Journal</i> , 2020, 118, 1076-1089.	0.2	3
1794	Selectivity filter modalities and rapid inactivation of the hERG1 channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 2795-2804.	3.3	31
1795	Design and analysis of polypeptide nanofiber using full atomistic Molecular Dynamic. <i>Journal of Molecular Liquids</i> , 2020, 302, 112610.	2.3	14

#	ARTICLE	IF	CITATIONS
1796	Identification of a Potential Zika Virus Inhibitor Targeting NS5 Methyltransferase Using Virtual Screening and Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 562-568.	2.5	14
1797	Embedding Methods for Quantum Chemistry: Applications from Materials to Life Sciences. <i>Journal of the American Chemical Society</i> , 2020, 142, 3281-3295.	6.6	81
1798	A dual apolipoprotein C-II mimeticâ€“apolipoprotein C-III antagonist peptide lowers plasma triglycerides. <i>Science Translational Medicine</i> , 2020, 12, .	5.8	56
1799	Microscopic Characterization of GRP1 PH Domain Interaction with Anionic Membranes. <i>Journal of Computational Chemistry</i> , 2020, 41, 489-499.	1.5	29
1800	Crystal structure of human endothelin ETB receptor in complex with sarafotoxin S6b. <i>Biochemical and Biophysical Research Communications</i> , 2020, 528, 383-388.	1.0	19
1801	Structural basis of second-generation HIV integrase inhibitor action and viral resistance. <i>Science</i> , 2020, 367, 806-810.	6.0	73
1802	Pairwise-additive and polarizable atomistic force fields for molecular dynamics simulations of proteins. <i>Progress in Molecular Biology and Translational Science</i> , 2020, 170, 1-71.	0.9	16
1803	The nuclear Overhauser Effect (NOE) as a tool to study macromolecular confinement: Elucidation and disentangling of crowding and encapsulation effects. <i>Journal of Chemical Physics</i> , 2020, 152, 024120.	1.2	1
1804	Zipper-Like Unfolding of dsDNA Caused by Graphene Wrinkles. <i>Journal of Physical Chemistry C</i> , 2020, 124, 3332-3340.	1.5	11
1805	Molecular Simulation of Mechanical Properties and Membrane Activities of the ESCRT-III Complexes. <i>Biophysical Journal</i> , 2020, 118, 1333-1343.	0.2	14
1806	System Size Dependence of Hydration-Shell Occupancy and Its Implications for Assessing the Hydrophobic and Hydrophilic Contributions to Hydration. <i>Journal of Physical Chemistry B</i> , 2020, 124, 798-806.	1.2	8
1807	A Structural Study on the <i>Listeria Monocytogenes</i> Internalin Aâ€”Human E-cadherin Interaction: A Molecular Tool to Investigate the Effects of Missense Mutations. <i>Toxins</i> , 2020, 12, 60.	1.5	7
1808	<i>Alternaria</i> toxins as casein kinase 2 inhibitors and possible consequences for estrogenicity: a hybrid in silico/in vitro study. <i>Archives of Toxicology</i> , 2020, 94, 2225-2237.	1.9	19
1809	Discovery, Optimization, and Characterization of ML417: A Novel and Highly Selective D ₃ Dopamine Receptor Agonist. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 5526-5567.	2.9	15
1810	Variance of Atomic Coordinates as a Dynamical Metric to Distinguish Proteins and Proteinâ€”Protein Interactions in Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2020, 124, 4247-4262.	1.2	4
1811	Structural and Functional Analysis of Gly212 Mutants Reveals the Importance of Intersubunit Interactions in ASIC1a Channel Function. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 58.	1.6	9
1812	Mechanistic insights into the crucial roles of Glu76 residue in nickel-dependent quercetin 2,4-dioxygenase for quercetin oxidative degradation. <i>Journal of Catalysis</i> , 2020, 387, 73-83.	3.1	3
1813	Inter-domain dynamics in the chaperone SurA and multi-site binding to its outer membrane protein clients. <i>Nature Communications</i> , 2020, 11, 2155.	5.8	48

#	ARTICLE	IF	CITATIONS
1814	Human CYP2E1-activated mutagenicity of dioxin-like PCBs 105 and 118â€”Experimental data consistent with molecular docking results. <i>Toxicology</i> , 2020, 437, 152438.	2.0	13
1815	Rational Design of Mixed Solvent Systems for Acid-Catalyzed Biomass Conversion Processes Using a Combined Experimental, Molecular Dynamics and Machine Learning Approach. <i>Topics in Catalysis</i> , 2020, 63, 649-663.	1.3	11
1816	Nicotinamide reduces inflammation and oxidative stress via the cholinergic system in fructose-induced metabolic syndrome in rats. <i>Life Sciences</i> , 2020, 250, 117585.	2.0	13
1817	¹³ C NMR Relaxation Analysis of Protein GB3 for the Assessment of Side Chain Dynamics Predictions by Current AMBER and CHARMM Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2896-2913.	2.3	14
1818	Further Optimization and Validation of the Classical Drude Polarizable Protein Force Field. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3221-3239.	2.3	53
1819	Truncated (N)-Methanocarba Nucleosides as Partial Agonists at Mouse and Human A ₃ Adenosine Receptors: Affinity Enhancement by <i>N</i> ⁶ -(2-Phenylethyl) Substitution. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 4334-4348.	2.9	17
1820	Investigation of the Drug Resistance Mechanism of M2-S31N Channel Blockers through Biomolecular Simulations and Viral Passage Experiments. <i>ACS Pharmacology and Translational Science</i> , 2020, 3, 666-675.	2.5	17
1821	Structural insights into tetraspanin CD9 function. <i>Nature Communications</i> , 2020, 11, 1606.	5.8	114
1822	Dynamic plasticity of the lipid antigen-binding site of CD1d is crucially favoured by acidic pH and helper proteins. <i>Scientific Reports</i> , 2020, 10, 5714.	1.6	4
1823	Structural Dynamics of the Lipid Antigen-Binding Site of CD1d Protein. <i>Biomolecules</i> , 2020, 10, 532.	1.8	4
1824	An In Silico Target Fishing Approach to Identify Novel Ochratoxin A Hydrolyzing Enzyme. <i>Toxins</i> , 2020, 12, 258.	1.5	18
1825	Exploiting a Mechanical Perturbation of a Titin Domain to Identify How Force Field Parameterization Affects Protein Refolding Pathways. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3240-3252.	2.3	5
1826	Perturbâ€“Pull: A Novel Method Facilitating Conformational Transitions in Proteins. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3825-3841.	2.3	26
1827	Predicting Reactive Cysteines with Implicit-Solvent-Based Continuous Constant pH Molecular Dynamics in Amber. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3689-3698.	2.3	30
1828	Anti-HIV drug repurposing against SARS-CoV-2. <i>RSC Advances</i> , 2020, 10, 15775-15783.	1.7	76
1829	Structural Explanations of Flavin Adenine Dinucleotide Binding in <i>Drosophila melanogaster</i> Cryptochrome. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3866-3870.	2.1	9
1830	Structural basis of ER-associated protein degradation mediated by the Hrd1 ubiquitin ligase complex. <i>Science</i> , 2020, 368, .	6.0	143
1831	Probing the effect of polyethylene glycol on the adsorption mechanisms of Gem on the hexagonal boron nitride as a highly efficient polymer-based drug delivery system: DFT, classical MD and Well-tempered Metadynamics simulations. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 98, 107613.	1.3	21

#	ARTICLE	IF	CITATIONS
1832	The Role of Electrostatics in Enzymes: Do Biomolecular Force Fields Reflect Protein Electric Fields?. Journal of Chemical Information and Modeling, 2020, 60, 3131-3144.	2.5	29
1833	Comparison of the Performance of Machine Learning Models in Representing High-Dimensional Free Energy Surfaces and Generating Observables. Journal of Physical Chemistry B, 2020, 124, 3647-3660.	1.2	20
1834	Role of Asp190 in the Phosphorylation of the Antibiotic Kanamycin Catalyzed by the Aminoglycoside Phosphotransferase Enzyme: A Combined QM:QM and MD Study. Journal of Physical Chemistry B, 2020, 124, 3494-3504.	1.2	5
1835	Free Energy Analysis of a Conformational Change of Heme ABC Transporter BhuUV-T. Journal of Physical Chemistry Letters, 2020, 11, 2824-2829.	2.1	9
1836	Structural Phylogenetics with Confidence. Molecular Biology and Evolution, 2020, 37, 2711-2726.	3.5	8
1837	Phase-plate cryo-EM structure of the Widom 601 CENP-A nucleosome core particle reveals differential flexibility of the DNA ends. Nucleic Acids Research, 2020, 48, 5735-5748.	6.5	27
1838	Human CYP2E1-dependent mutagenicity of benzene and its hydroxylated metabolites in V79 derived cells: Suppression and enhancement by ethanol pretreatment. Environmental and Molecular Mutagenesis, 2020, 61, 622-634.	0.9	6
1839	Structural dynamics of inosine triphosphate pyrophosphatase (ITPA) protein and two clinically relevant mutants: molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1236-1247.	2.0	5
1840	Characterization of VopJ by modelling, docking and molecular dynamics simulation with reference to its role in infection of enteropathogen Vibrio parahaemolyticus. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1572-1578.	2.0	2
1841	Molecular Dynamics Simulation of Biomolecular Interactions. , 2021, , 182-189.		9
1842	Using a viral 2A peptide-based strategy to reconstruct the bovine P450scc steroidogenic system in S. cerevisiae. Journal of Biotechnology, 2021, 325, 186-195.	1.9	4
1843	NMR Structure and Dynamics Studies of Yeast Respiratory Supercomplex Factor 2. Structure, 2021, 29, 275-283.e4.	1.6	10
1844	Toward Biotherapeutics Formulation Composition Engineering using Site-Identification by Ligand Competitive Saturation (SILCS). Journal of Pharmaceutical Sciences, 2021, 110, 1103-1110.	1.6	9
1845	Annexin A4 trimers are recruited by high membrane curvatures in giant plasma membrane vesicles. Soft Matter, 2021, 17, 308-318.	1.2	28
1846	Passive Internalization of Bioactive β -Casein Peptides into Phospholipid (POPC) Bilayers. Free Energy Landscapes from Unbiased Equilibrium MD Simulations at $\frac{1}{4}$ s-Time Scale. Food Biophysics, 2021, 16, 70-83.	1.4	0
1847	Fusion peptide engineered electrostatically-versatile titanium implant simultaneously enhancing anti-infection, vascularization and osseointegration. Biomaterials, 2021, 264, 120446.	5.7	52
1848	Conformational stability of the bacterial adhesin, FimH , with an inactivating mutation. Proteins: Structure, Function and Bioinformatics, 2021, 89, 276-288.	1.5	6
1849	Domain focused and residue focused phosphorylation effect on tau protein: A molecular dynamics simulation study. Journal of the Mechanical Behavior of Biomedical Materials, 2021, 113, 104149.	1.5	13

#	ARTICLE	IF	CITATIONS
1850	Temperature dependent aggregation mechanism and pathway of lysozyme: By all atom and coarse grained molecular dynamics simulation. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 103, 107816.	1.3	3
1851	A lightweight method for evaluating in situ workflow efficiency. <i>Journal of Computational Science</i> , 2021, 48, 101259.	1.5	7
1852	Structure based peptide design, molecular dynamics and MM-PBSA studies for targeting C terminal dimerization of NFAT5 DNA binding domain. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 103, 107804.	1.3	6
1853	Dynamics of an LPS translocon induced by substrate and an antimicrobial peptide. <i>Nature Chemical Biology</i> , 2021, 17, 187-195.	3.9	41
1854	Molecular mechanism of inhibiting the SARS-CoV-2 cell entry facilitator TMPRSS2 with camostat and nafamostat. <i>Chemical Science</i> , 2021, 12, 983-992.	3.7	66
1855	Update of CHARMM36's atomic charges for aromatic amino acids in water solution simulations and spectroscopy analysis via sequential molecular dynamics and DFT calculations. <i>Journal of Molecular Liquids</i> , 2021, 321, 114739.	2.3	12
1856	Further thermo-stabilization of thermophilic rhodopsin from <i>Thermus thermophilus</i> through engineering in extramembrane regions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 301-310.	1.5	6
1857	Predicting Genetic Variation Severity Using Machine Learning to Interpret Molecular Simulations. <i>Biophysical Journal</i> , 2021, 120, 189-204.	0.2	15
1858	Interplay of cholesterol, membrane bilayers and the AT1R: A cholesterol consensus motif on AT1R is revealed. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 110-120.	1.9	7
1859	Survivin - caspase protein-protein interaction: Experimental evidence and computational investigations to decipher the hotspot residues for drug targeting. <i>Journal of Molecular Structure</i> , 2021, 1229, 129619.	1.8	8
1860	Hydroxylated Chalcones as Aryl Hydrocarbon Receptor Agonists: Structure-Activity Effects. <i>Toxicological Sciences</i> , 2021, 180, 148-159.	1.4	2
1861	Interactions of zinc aqua complexes with ovalbumin at the forefront of the Zn ²⁺ /ZnO-OVO hybrid complex formation mechanism. <i>Applied Surface Science</i> , 2021, 542, 148641.	3.1	16
1862	Cyclodipeptide Synthases of the NYH Subfamily Recognize tRNA Using an Î±-Helix Enriched with Positive Residues. <i>Biochemistry</i> , 2021, 60, 64-76.	1.2	0
1863	Enhancing Cationic Drug Delivery with Polymeric Carriers: The Coulomb-pH Switch Approach. <i>Advanced Theory and Simulations</i> , 2021, 4, 2000247.	1.3	1
1864	N-Terminus of the Third PDZ Domain of PSD-95 Orchestrates Allosteric Communication for Selective Ligand Binding. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 347-357.	2.5	2
1865	Molecular dynamic simulations, ¹³ C-NMR and TD-DFT spectroscopy analyze for zwitterionic isoleucine (<i>ILE</i>) _N , 1- <i>ILE</i> _N , in water solution. <i>Journal of Computational Chemistry</i> , 2021, 42, 344-357.		
1866	Unraveling the origin of interactions of hydroxychloroquine with the receptor-binding domain of SARS-CoV-2 in aqueous medium. <i>Chemical Physics Letters</i> , 2021, 764, 138280.	1.2	1
1867	Structural Characterization and Modeling of a Respiratory Syncytial Virus Fusion Glycoprotein Nanoparticle Vaccine in Solution. <i>Molecular Pharmaceutics</i> , 2021, 18, 359-376.	2.3	12

#	ARTICLE	IF	CITATIONS
1868	Modeling Shows that Rotation about the Peroxide O-O Bond Assists Protein and Lipid Functional Groups in Discriminating between H ₂ O ₂ and H ₂ O. <i>Journal of Physical Chemistry B</i> , 2021, 125, 137-147.	1.2	2
1869	A multiscale coarse-grained model of the SARS-CoV-2 virion. <i>Biophysical Journal</i> , 2021, 120, 1097-1104.	0.2	139
1870	A Framework Nucleic Acid Based Robotic Nanobee for Active Targeting Therapy. <i>Advanced Functional Materials</i> , 2021, 31, 2007342.	7.8	65
1871	Similarities and Differences between Crystal and Enzyme Environmental Effects on the Electron Density of Drug Molecules. <i>Chemistry - A European Journal</i> , 2021, 27, 3407-3419.	1.7	10
1872	Residues flanking the ARKme3T/S motif allow binding of diverse targets to the HP1 chromodomain: Insights from molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2021, 1865, 129771.	1.1	2
1873	A detailed picture of a protein-carbohydrate hydrogen-bonding network revealed by NMR and MD simulations. <i>Glycobiology</i> , 2021, 31, 508-518.	1.3	6
1874	Computational design of SARS-CoV-2 spike glycoproteins to increase immunogenicity by T cell epitope engineering. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 518-529.	1.9	19
1876	Kinetic and thermodynamic stability comparison for the fibrillar form of small amyloid- β (1-42) oligomers using scaled molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16897-16908.	1.3	3
1877	Accurate protein structure prediction with hydroxyl radical protein footprinting data. <i>Nature Communications</i> , 2021, 12, 341.	5.8	31
1878	A simplified charge projection scheme for long-range electrostatics in <i>ab initio</i> QM/MM calculations. <i>Journal of Chemical Physics</i> , 2021, 154, 024115.	1.2	18
1879	Updating atomic charge parameters of aliphatic amino acids: a quest to improve the performance of molecular modeling <i>via</i> sequential molecular dynamics and DFT-GIAO-NMR calculations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8413-8425.	1.3	12
1881	The key role of the central cavity in sodium transport through ligand-gated two-pore channels. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18461-18474.	1.3	7
1882	HIV-1 Env-Dependent Cell Killing by Bifunctional Small-Molecule/Peptide Conjugates. <i>ACS Chemical Biology</i> , 2021, 16, 193-204.	1.6	4
1883	Using multiscale molecular dynamics simulations to obtain insights into pore forming toxin mechanisms. <i>Methods in Enzymology</i> , 2021, 649, 461-502.	0.4	9
1884	Small molecules inhibitors of the heterogeneous ribonuclear protein A18 (hnRNP A18): a regulator of protein translation and an immune checkpoint. <i>Nucleic Acids Research</i> , 2021, 49, 1235-1246.	6.5	10
1885	Genotype & phenotype in Lowe Syndrome: specific <i>OCRL1</i> patient mutations differentially impact cellular phenotypes. <i>Human Molecular Genetics</i> , 2021, 30, 198-212.	1.4	8
1886	Binding of azobenzene and <i>p</i> -diaminoazobenzene to the human voltage-gated sodium channel Na _v 1.4. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 3552-3564.	1.3	13
1887	The structural changes in the signaling mechanism of bacteriophytochromes in solution revealed by a multiscale computational investigation. <i>Chemical Science</i> , 2021, 12, 5555-5565.	3.7	8

#	ARTICLE	IF	CITATIONS
1888	Molecular dynamics investigation on the interaction of human angiotensin-converting enzyme with tetrapeptide inhibitors. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6685-6694.	1.3	6
1889	Specificity of Molecular Fragments Binding to S100B versus S100A1 as Identified by NMR and Site Identification by Ligand Competitive Saturation (SILCS). <i>Molecules</i> , 2021, 26, 381.	1.7	6
1890	A double bilayer to study the nonequilibrium environmental response of GIRK2 in complex states. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15784-15795.	1.3	1
1891	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.	2.3	46
1892	Recent advances in atomic molecular dynamics simulation of intrinsically disordered proteins. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 777-784.	1.3	45
1893	Structural basis for voltage-sensor trapping of the cardiac sodium channel by a deathstalker scorpion toxin. <i>Nature Communications</i> , 2021, 12, 128.	5.8	54
1894	Model of the RNA Polymerase Complex of the SARS-CoV-2 Virus with Favipiravir. <i>Russian Journal of Physical Chemistry B</i> , 2021, 15, 103-107.	0.2	3
1895	Structure-Based Modeling of Complement C4 Mediated Neutralization of Adenovirus. <i>Viruses</i> , 2021, 13, 111.	1.5	2
1897	Mechanism of the feedback-inhibition resistance in aspartate kinase of <i>Corynebacterium pekinense</i> : from experiment to MD simulations. <i>RSC Advances</i> , 2021, 11, 30-38.	1.7	2
1898	Repurposing FDA-approved drugs to fight COVID-19 using in silico methods: Targeting SARS-CoV-2 RdRp enzyme and host cell receptors (ACE2, CD147) through virtual screening and molecular dynamic simulations. <i>Informatics in Medicine Unlocked</i> , 2021, 23, 100541.	1.9	24
1899	Stepwise gating of the Sec61 protein-conducting channel by Sec63 and Sec62. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 162-172.	3.6	43
1900	Phosphorothioate Substitutions in RNA Structure Studied by Molecular Dynamics Simulations, QM/MM Calculations, and NMR Experiments. <i>Journal of Physical Chemistry B</i> , 2021, 125, 825-840.	1.2	11
1901	Identification of vaccine candidate proteins in <i>Ureaplasma urealyticum</i> causing infertility. <i>Indian Journal of Sexually Transmitted Diseases and AIDS</i> , 2021, 42, 95-100.	0.1	1
1902	Conserved binding site in the N-lobe of prokaryotic MATE transporters suggests a role for Na ⁺ in ion-coupled drug efflux. <i>Journal of Biological Chemistry</i> , 2021, 296, 100262.	1.6	8
1903	Structures of the archaerhodopsin-3 transporter reveal that disordering of internal water networks underpins receptor sensitization. <i>Nature Communications</i> , 2021, 12, 629.	5.8	22
1904	Multiscale modeling shows that dielectric differences make NaV channels faster than KV channels. <i>Journal of General Physiology</i> , 2021, 153, .	0.9	11
1905	Structure-guided evolution of a ketoreductase for efficient and stereoselective bioreduction of bulky 1 ^o -amino 2 ^o -keto esters. <i>Catalysis Science and Technology</i> , 2021, 11, 6755-6769.	2.1	8
1906	On the chirality-dependent adsorption behavior of volatile organic compounds on carbon nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21941-21950.	1.3	10

#	ARTICLE	IF	CITATIONS
1907	Chemical Changes of Wood Treated with Caffeine. <i>Materials</i> , 2021, 14, 497.	1.3	17
1908	Using yeast two-hybrid system and molecular dynamics simulation to detect venom protein-protein interactions. <i>Current Research in Toxicology</i> , 2021, 2, 93-98.	1.3	4
1909	Folding and self-assembly of short intrinsically disordered peptides and protein regions. <i>Nanoscale Advances</i> , 2021, 3, 1789-1812.	2.2	15
1910	Qualitative Prediction of Ligand Dissociation Kinetics from Focal Adhesion Kinase Using Steered Molecular Dynamics. <i>Life</i> , 2021, 11, 74.	1.1	14
1911	Poor Personâ€™s pH Simulation of Membrane Proteins. <i>Methods in Molecular Biology</i> , 2021, 2315, 197-217.	0.4	1
1912	Molecular basis for the adaptive evolution of environment-sensing by H-NS proteins. <i>ELife</i> , 2021, 10, .	2.8	9
1913	Systematic Differences between Current Molecular Dynamics Force Fields To Represent Local Properties of Intrinsically Disordered Proteins. <i>Journal of Physical Chemistry B</i> , 2021, 125, 798-804.	1.2	18
1914	Calmodulin complexes with brain and muscle creatine kinase peptides. <i>Current Research in Structural Biology</i> , 2021, 3, 121-132.	1.1	5
1915	<i>In silico</i> design of peptides with binding to the receptor binding domain (RBD) of the SARS-CoV-2 and their utility in bio-sensor development for SARS-CoV-2 detection. <i>RSC Advances</i> , 2021, 11, 3816-3826.	1.7	17
1916	Covalent and non-covalent binding free energy calculations for peptidomimetic inhibitors of SARS-CoV-2 main protease. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6746-6757.	1.3	30
1917	Self-assembly, interfacial properties, interactions with macromolecules and molecular modelling and simulation of microbial bio-based amphiphiles (biosurfactants). A tutorial review. <i>Green Chemistry</i> , 2021, 23, 3842-3944.	4.6	61
1918	SARS-CoV-2 spike protein N501Y mutation causes differential species transmissibility and antibody sensitivity: a molecular dynamics and alchemical free energy study. <i>Molecular Systems Design and Engineering</i> , 2021, 6, 964-974.	1.7	8
1919	Membrane models for molecular simulations of peripheral membrane proteins. <i>Advances in Physics: X</i> , 2021, 6, 1932589.	1.5	3
1920	Local Bilayer Hydrophobicity Modulates Membrane Protein Stability. <i>Journal of the American Chemical Society</i> , 2021, 143, 764-772.	6.6	21
1923	Controlling opioid receptor functional selectivity by targeting distinct subpockets of the orthosteric site. <i>ELife</i> , 2021, 10, .	2.8	40
1924	Deciphering the Mechanism of Inhibition of SERCA1a by Sarcolipin Using Molecular Simulations. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 606254.	1.6	4
1925	Altered structure and dynamics of pathogenic cytochrome <i>c</i> variants correlate with increased apoptotic activity. <i>Biochemical Journal</i> , 2021, 478, 669-684.	1.7	8
1926	Glutamate transporters have a chloride channel with two hydrophobic gates. <i>Nature</i> , 2021, 591, 327-331.	13.7	40

#	ARTICLE	IF	CITATIONS
1927	Design of immunogens to elicit broadly neutralizing antibodies against HIV targeting the CD4 binding site. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	6
1928	Computationally-obtained structural insights into the molecular interactions between Pidilizumab and binding partners DLL1 and PD-1. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-13.	2.0	2
1929	The Interplay of Ligand Properties and Core Size Dictates the Hydrophobicity of Monolayer-Protected Gold Nanoparticles. <i>ACS Nano</i> , 2021, 15, 4534-4545.	7.3	22
1930	Temperature-Dependent Kinetic Isotope Effects in R67 Dihydrofolate Reductase from Path-Integral Simulations. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1369-1377.	1.2	8
1932	Transition Path Sampling Study of the Feruloyl Esterase Mechanism. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2018-2030.	1.2	11
1933	Polarization Effects in Water-Mediated Selective Cation Transport across a Narrow Transmembrane Channel. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1726-1741.	2.3	26
1934	Sertaconazole induced toxicity in HeLa cells through mitotic arrest and inhibition of microtubule assembly. <i>Naunyn-Schmiedeberg's Archives of Pharmacology</i> , 2021, 394, 1231-1249.	1.4	9
1935	Molecular simulations of lipid membrane partitioning and translocation by bacterial quorum sensing modulators. <i>PLoS ONE</i> , 2021, 16, e0246187.	1.1	13
1938	Dissecting Role of Charged Residue from Transmembrane Domain 5 of Latent Membrane Protein 1 via In Silico Simulations and Wet-Lab Experiments. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2124-2133.	1.2	1
1939	Membrane fouling by lysozyme: Effect of local interaction. <i>AIChE Journal</i> , 2021, 67, e17212.	1.8	12
1940	Dynamic Community Composition Unravels Allosteric Communication in PDZ3. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2266-2276.	1.2	8
1942	Structural Mechanism of \bar{I} -Currents in a Mutated Kv7.2 Voltage Sensor Domain from Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1354-1367.	2.5	6
1943	On the Role of a Conserved Methionine in the Na ⁺ -Coupling Mechanism of a Neurotransmitter Transporter Homolog. <i>Neurochemical Research</i> , 2021, , 1.	1.6	4
1944	Glycan Cluster Shielding and Antibody Epitopes on Lassa Virus Envelop Protein. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2089-2097.	1.2	6
1945	Novel $\hat{\pm}$ -amylase and $\hat{\pm}$ -glucosidase inhibitors from selected Nigerian antidiabetic plants: an <i>in silico</i> approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 6340-6349.	2.0	11
1947	Analyzing the driving forces of insulin stability in the basic amino acid solutions: A perspective from hydration dynamics. <i>Journal of Chemical Physics</i> , 2021, 154, 084901.	1.2	5
1948	Development and Validation of a DFT-Based Force Field for a Hydrated Homoalanine Polypeptide. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1568-1581.	1.2	6
1949	Investigation of the aquaporin $\hat{2}$ gating mechanism with molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 819-831.	1.5	18

#	ARTICLE	IF	CITATIONS
1950	Structural basis of diversity and homodimerization specificity of zinc-finger-associated domains in <i>Drosophila</i> . <i>Nucleic Acids Research</i> , 2021, 49, 2375-2389.	6.5	17
1951	Frontiers in Multiscale Modeling of Photoreceptor Proteins. <i>Photochemistry and Photobiology</i> , 2021, 97, 243-269.	1.3	26
1952	How μ -opioid receptor recognizes fentanyl. <i>Nature Communications</i> , 2021, 12, 984.	5.8	56
1955	Inhibition Mechanism of Antimalarial Drugs Targeting the Cytochrome bc ₁ Complex. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1334-1345.	2.5	5
1956	Structural Basis for the Function of the C-Terminal Proton Release Pathway in the Calcium Pump. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3507.	1.8	0
1957	Light-Induced Change of Arginine Conformation Modulates the Rate of Adenosine Triphosphate to Cyclic Adenosine Monophosphate Conversion in the Optogenetic System Containing Photoactivated Adenylyl Cyclase. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1215-1225.	2.5	13
1958	Comparison of Carbohydrate Force Fields in Molecular Dynamics Simulations of Protein-Carbohydrate Complexes. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2575-2585.	2.3	23
1959	Early-stage dynamics of chloride ion-pumping rhodopsin revealed by a femtosecond X-ray laser. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	41
1960	Beta-1,3 Oligoglucans Specifically Bind to Immune Receptor CD28 and May Enhance T Cell Activation. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3124.	1.8	6
1961	Resin-acid derivatives bind to multiple sites on the voltage-sensor domain of the Shaker potassium channel. <i>Journal of General Physiology</i> , 2021, 153, .	0.9	2
1962	Targeting the transmembrane domain 5 of latent membrane protein 1 using small molecule modulators. <i>European Journal of Medicinal Chemistry</i> , 2021, 214, 113210.	2.6	2
1963	Intranasal fusion inhibitory lipopeptide prevents direct-contact SARS-CoV-2 transmission in ferrets. <i>Science</i> , 2021, 371, 1379-1382.	6.0	158
1964	ABCG2 Is Overexpressed on Red Blood Cells in Ph-Negative Myeloproliferative Neoplasms and Potentiates Ruxolitinib-Induced Apoptosis. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3530.	1.8	3
1965	A rational design of a multi-epitope vaccine against SARS-CoV-2 which accounts for the glycan shield of the spike glycoprotein. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 7099-7113.	2.0	15
1966	Overexpression of an Agave Phosphoenolpyruvate Carboxylase Improves Plant Growth and Stress Tolerance. <i>Cells</i> , 2021, 10, 582.	1.8	24
1967	Structural insights into membrane remodeling by SNX1. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	11
1968	Multi-Scale Flexible Fitting of Proteins to Cryo-EM Density Maps at Medium Resolution. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 631854.	1.6	13
1969	Lipid regulation of hERG1 channel function. <i>Nature Communications</i> , 2021, 12, 1409.	5.8	9

#	ARTICLE	IF	CITATIONS
1970	Impact of surface state on polyethylene glycol conformation confined inside a nanopore. <i>Journal of Chemical Physics</i> , 2021, 154, 104901.	1.2	6
1971	Coupling Monte Carlo, Variational Implicit Solvation, and Binary Level-Set for Simulations of Biomolecular Binding. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2465-2478.	2.3	6
1972	How does Sec63 affect the conformation of Sec61 in yeast?. <i>PLoS Computational Biology</i> , 2021, 17, e1008855.	1.5	13
1974	The Morphology of Hydroxyapatite Nanoparticles Regulates Cargo Recognition in Clathrin-Mediated Endocytosis. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 627015.	1.6	13
1975	All-Atom MD Simulations of the HBV Capsid Complexed with AT130 Reveal Secondary and Tertiary Structural Changes and Mechanisms of Allostery. <i>Viruses</i> , 2021, 13, 564.	1.5	15
1976	Molecular Basis of Class B GPCR Selectivity for the Neuropeptides PACAP and VIP. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 644644.	1.6	15
1977	Chloride-dependent conformational changes in the GlyT1 glycine transporter. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	16
1979	Implicit Solvents for the Polarizable Atomic Multipole AMOEBA Force Field. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2323-2341.	2.3	10
1980	Searching for Aquamelt Behavior among Silklike Biomimetics during Fibrillation under Flow. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3238-3250.	1.2	1
1981	Elusive Intermediate State Key in the Conversion of ATP Hydrolysis into Useful Work Driving the Ca ²⁺ Pump SERCA. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2921-2928.	1.2	3
1982	Mutational fitness landscapes reveal genetic and structural improvement pathways for a vaccine-elicited HIV-1 broadly neutralizing antibody. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	21
1983	Elucidation of interactions regulating conformational stability and dynamics of SARS-CoV-2 S-protein. <i>Biophysical Journal</i> , 2021, 120, 1060-1071.	0.2	57
1985	CENP-A Nucleosome is a Sensitive Allosteric Scaffold for DNA and Chromatin Factors. <i>Journal of Molecular Biology</i> , 2021, 433, 166789.	2.0	5
1986	Atomic-Resolution 1.3 Å... Crystal Structure, Inhibition by Sulfate, and Molecular Dynamics of the Bacterial Enzyme DapE. <i>Biochemistry</i> , 2021, 60, 908-917.	1.2	6
1987	MLLPA : A Machine Learning-assisted Python module to study phase-specific events in lipid membranes. <i>Journal of Computational Chemistry</i> , 2021, 42, 930-943.	1.5	3
1988	Xanthone glucoside 2-β-D-glucopyranosyl-1,3,6,7-tetrahydroxy-9H-xanthen-9-one binds to the ATP-binding pocket of glycogen synthase kinase 3β and inhibits its activity: implications in prostate cancer and associated cardiovascular disease risk. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 7868-7884.	2.0	3
1989	Structure-Activity Relationship of Heterocyclic P2Y ₁₄ Receptor Antagonists: Removal of the Zwitterionic Character with Piperidine Bioisosteres. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 5099-5122.	2.9	11
1990	Defective internal allosteric network imparts dysfunctional ATP/substrate-binding cooperativity in oncogenic chimera of protein kinase A. <i>Communications Biology</i> , 2021, 4, 321.	2.0	21

#	ARTICLE	IF	CITATIONS
1991	Exploring the new potential antiviral constituents of <i>Moringa oleifera</i> for SARS-COV-2 pathogenesis: An in silico molecular docking and dynamic studies. <i>Chemical Physics Letters</i> , 2021, 767, 138379.	1.2	58
1992	Kirkwood's Buff-Derived Force Field for Peptides and Proteins: Applications of KBFF20. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2991-3009.	2.3	6
1993	Ketamine Metabolite (2 <i>R</i> ,6 <i>R</i>)-Hydroxynorketamine Interacts with μ and κ Opioid Receptors. <i>ACS Chemical Neuroscience</i> , 2021, 12, 1487-1497.	1.7	13
1994	The RIT1 C-terminus associates with lipid bilayers via charge complementarity. <i>Computational Biology and Chemistry</i> , 2021, 91, 107437.	1.1	6
1995	Informing NMR experiments with molecular dynamics simulations to characterize the dominant activated state of the KcsA ion channel. <i>Journal of Chemical Physics</i> , 2021, 154, 165102.	1.2	11
1996	Lipophilicity of Cationic Ligands Promotes Irreversible Adsorption of Nanoparticles to Lipid Bilayers. <i>ACS Nano</i> , 2021, 15, 6562-6572.	7.3	27
1997	Effect of Stapling on the Thermodynamics of mdm2-p53 Binding. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1989-2000.	2.5	8
1999	A structural signature motif enlightens the origin and diversification of nuclear receptors. <i>PLoS Genetics</i> , 2021, 17, e1009492.	1.5	8
2000	Validation by Molecular Dynamics of the Major Components of Sugarcane Vinasse, On a Surface of Calcium Carbonate (Calcite). <i>Molecules</i> , 2021, 26, 2353.	1.7	2
2001	Origins of Clustering of Metalate-Extractant Complexes in Liquid-Liquid Extraction. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 24194-24206.	4.0	27
2002	Location and Conformational Ensemble of Menaquinone and Menaquinol, and Protein-Lipid Modulations in Archaeal Membranes. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4714-4725.	1.2	10
2003	Integrated Biophysical Modeling of the SARS-CoV-2 Spike Protein Binding and Allosteric Interactions with Antibodies. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4596-4619.	1.2	60
2005	Mesoscale Simulation of Bacterial Chromosome and Cytoplasmic Nanoparticles in Confinement. <i>Entropy</i> , 2021, 23, 542.	1.1	1
2006	Charge-Free, Stabilizing Amide-Hydrogen Interactions Can Be Used to Control Collagen Triple-Helix Self-Assembly. <i>Biomacromolecules</i> , 2021, 22, 2137-2147.	2.6	16
2007	Boronic Acids as Prospective Inhibitors of Metallo- β -Lactamases: Efficient Chemical Reaction in the Enzymatic Active Site Revealed by Molecular Modeling. <i>Molecules</i> , 2021, 26, 2026.	1.7	11
2008	Viscoelastic Response of Neurofilaments: An Atomistic Simulation Approach. <i>Biomolecules</i> , 2021, 11, 540.	1.8	6
2009	Synthesis, Biological Activity, and Molecular Dynamics Study of Novel Series of a Trimethoprim Analogs as Multi-Targeted Compounds: Dihydrofolate Reductase (DHFR) Inhibitors and DNA-Binding Agents. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3685.	1.8	19
2011	Long-Time-Scale Predictions from Short-Trajectory Data: A Benchmark Analysis of the Trp-Cage Miniprotein. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2948-2963.	2.3	20

#	ARTICLE	IF	CITATIONS
2012	Structure of HIV-1 gp41 with its membrane anchors targeted by neutralizing antibodies. <i>ELife</i> , 2021, 10, .	2.8	15
2013	An in vitro study on the transport and phase II metabolism of the mycotoxin alternariol in combination with the structurally related gut microbial metabolite urolithin C. <i>Toxicology Letters</i> , 2021, 340, 15-22.	0.4	11
2014	How adding a single methylene to dihydrofolate reductase can change its conformational dynamics. <i>Journal of Chemical Physics</i> , 2021, 154, 165103.	1.2	2
2015	Atomistic dynamics of a viral infection process: Release of membrane lytic peptides from a non-enveloped virus. <i>Science Advances</i> , 2021, 7, .	4.7	6
2016	The binding mechanism of ivermectin and levosalbutamol with spike protein of SARS-CoV-2. <i>Structural Chemistry</i> , 2021, 32, 1985-1992.	1.0	18
2017	Exploring the Minimum-Energy Pathways and Free-Energy Profiles of Enzymatic Reactions with QM/MM Calculations. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4701-4713.	1.2	21
2018	Rare germline variants in the E-cadherin gene CDH1 are associated with the risk of brain tumors of neuroepithelial and epithelial origin. <i>Acta Neuropathologica</i> , 2021, 142, 191-210.	3.9	6
2019	Biomolecular interaction mechanism of an anticancer drug, pazopanib with human serum albumin: a multi-spectroscopic and computational approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 8312-8323.	2.0	3
2020	A strategy for proline and glycine mutations to proteins with alchemical free energy calculations. <i>Journal of Computational Chemistry</i> , 2021, 42, 1088-1094.	1.5	12
2021	Dual nature of human ACE2 glycosylation in binding to SARS-CoV-2 spike. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	131
2023	Insights into Glucose-6-phosphate Allosteric Activation of Î ² -Glucosidase A. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1931-1941.	2.5	4
2024	Refinement of Î±-Synuclein Ensembles Against SAXS Data: Comparison of Force Fields and Methods. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 654333.	1.6	51
2025	The Importance of N186 in the Alpha-1-Antitrypsin Shutter Region Is Revealed by the Novel Bologna Deficiency Variant. <i>International Journal of Molecular Sciences</i> , 2021, 22, 5668.	1.8	5
2026	Parkinson Hastalıkları ile İlişkiliendirilen PreNAC Fibril Kesiti ve Onun A53C, A53E, A53G, A53T, A53V Mutasyonlarının Yapısal Kararlılığı Araştırılması. <i>SDU Journal of Science</i> , 0, , 66-76.	0.1	0
2027	Stressed Lipid Droplets: How Neutral Lipids Relieve Surface Tension and Membrane Expansion Drives Protein Association. <i>Journal of Physical Chemistry B</i> , 2021, 125, 5572-5586.	1.2	18
2028	Defining the Energetic Basis for a Conformational Switch Mediating Ligand-Independent Activation of Mutant Estrogen Receptors in Breast Cancer. <i>Molecular Cancer Research</i> , 2021, 19, 1559-1570.	1.5	6
2029	Piezoelectricity of the Transmembrane Protein <i>ba₃</i> Cytochrome <i>c</i> Oxidase. <i>Advanced Functional Materials</i> , 2021, 31, 2100884.	7.8	12
2030	Revealing the activation mechanism of autoinhibited RalF by integrated simulation and experimental approaches. <i>Scientific Reports</i> , 2021, 11, 10059.	1.6	5

#	ARTICLE	IF	CITATIONS
2031	ReFOLD3: refinement of 3D protein models with gradual restraints based on predicted local quality and residue contacts. <i>Nucleic Acids Research</i> , 2021, 49, W589-W596.	6.5	8
2032	Cryo-EM electron microscopy structure of the antidiuretic hormone arginine-vasopressin V2 receptor signaling complex. <i>Science Advances</i> , 2021, 7, .	4.7	25
2033	Mechanism of MRX inhibition by Rif2 at telomeres. <i>Nature Communications</i> , 2021, 12, 2763.	5.8	22
2034	Energetics and structure of alanine-rich α -helices via adaptive steered molecular dynamics. <i>Biophysical Journal</i> , 2021, 120, 2009-2018.	0.2	13
2035	Modeling the Energy Landscape of Side Reactions in the Cytochrome bc1 Complex. <i>Frontiers in Chemistry</i> , 2021, 9, 643796.	1.8	6
2036	Solution structure of deglycosylated human IgG1 shows the role of CH2 glycans in its conformation. <i>Biophysical Journal</i> , 2021, 120, 1814-1834.	0.2	3
2037	Molecular Docking and Dynamics Simulation Revealed the Potential Inhibitory Activity of ACEIs Against SARS-CoV-2 Targeting the hACE2 Receptor. <i>Frontiers in Chemistry</i> , 2021, 9, 661230.	1.8	122
2038	Gas-phase ion/ion chemistry for structurally sensitive probes of gaseous protein ion structure: Electrostatic and electrostatic to covalent cross-linking. <i>International Journal of Mass Spectrometry</i> , 2021, 463, 116549.	0.7	10
2039	Impact of PIP2 Lipids, Force Field Parameters, and Mutational Analysis on the Binding of the Osh4 TM s α -7 Domain. <i>Journal of Physical Chemistry B</i> , 2021, 125, 5296-5308.	1.2	1
2040	Critical Interactions Between the SARS-CoV-2 Spike Glycoprotein and the Human ACE2 Receptor. <i>Journal of Physical Chemistry B</i> , 2021, 125, 5537-5548.	1.2	41
2041	General Protocol for Constructing Molecular Models of Nanodiscs. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2869-2883.	2.5	11
2044	Channelrhodopsin C1C2: Photocycle kinetics and interactions near the central gate. <i>Biophysical Journal</i> , 2021, 120, 1835-1845.	0.2	2
2045	Replica Exchange Molecular Dynamics of Diphenylalanine Amyloid Peptides in Electric Fields. <i>Journal of Physical Chemistry B</i> , 2021, 125, 5233-5242.	1.2	5
2046	Structural Heterogeneity of Human Histone H2A.1. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4977-4986.	1.2	5
2047	Integrated support vector machine and pharmacophore based virtual screening driven identification of thiophene carboxamide scaffold containing compound as potential PARP1 inhibitor. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-14.	2.0	5
2048	Unusual mode of dimerization of retinitis pigmentosa-associated F220C rhodopsin. <i>Scientific Reports</i> , 2021, 11, 10536.	1.6	7
2049	Mapping the Intramolecular Communications among Different Glutamate Dehydrogenase States Using Molecular Dynamics. <i>Biomolecules</i> , 2021, 11, 798.	1.8	5
2050	Force Field Parameters for Fe ₂ +4S ²⁺ Clusters of Dihydropyrimidine Dehydrogenase, the 5-Fluorouracil Cancer Drug Deactivation Protein: A Step towards In Silico Pharmacogenomics Studies. <i>Molecules</i> , 2021, 26, 2929.	1.7	1

#	ARTICLE	IF	CITATIONS
2052	Protein Dynamics Is Altered by a High Surface Density of Atomic Transfer Radical Polymerization Polymers. <i>Langmuir</i> , 2021, 37, 7185-7193.	1.6	0
2053	Can molecular dynamics simulations improve the structural accuracy and virtual screening performance of GPCR models?. <i>PLoS Computational Biology</i> , 2021, 17, e1008936.	1.5	16
2054	Additive CHARMM36 Force Field for Nonstandard Amino Acids. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3554-3570.	2.3	39
2055	Conformational Reorganization of Apolipoprotein E Triggered by Phospholipid Assembly. <i>Journal of Physical Chemistry B</i> , 2021, 125, 5285-5295.	1.2	4
2056	Molecular dynamics investigation of the structural flexibility of H ₂ O ₂ and H ₂ S ₂ in response to medium polarity. <i>Journal of Molecular Liquids</i> , 2021, 329, 115469.	2.3	2
2057	Molecular dynamics study on membrane fouling by oppositely charged proteins. <i>AIChE Journal</i> , 2021, 67, e17335.	1.8	8
2058	Site-Selective Chemoenzymatic Modification on the Core Fucose of an Antibody Enhances Its Fcγ ₃ Receptor Affinity and ADCC Activity. <i>Journal of the American Chemical Society</i> , 2021, 143, 7828-7838.	6.6	17
2060	A potential solution to avoid overdose of mixed drugs in the event of Covid-19: Nanomedicine at the heart of the Covid-19 pandemic. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 104, 107834.	1.3	6
2061	Force Field Benchmark of Amino Acids. 3. Hydration with Scaled Lennard-Jones Interactions. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3571-3582.	2.5	15
2062	Rational design of antimicrobial peptides targeting Gram-negative bacteria. <i>Computational Biology and Chemistry</i> , 2021, 92, 107475.	1.1	4
2063	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. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7163-7176.	1.2	14
2064	Cyclodextrin solubilization in hydrated reline: Resolving the unique stabilization mechanism in a deep eutectic solvent. <i>Journal of Chemical Physics</i> , 2021, 154, 224505.	1.2	5
2065	Identification of potential antiviral compounds against SARS-CoV-2 structural and non structural protein targets: A pharmacoinformatics study of the CAS COVID-19 dataset. <i>Computers in Biology and Medicine</i> , 2021, 133, 104364.	3.9	6
2066	Crystal structure of an archaeal CorB magnesium transporter. <i>Nature Communications</i> , 2021, 12, 4028.	5.8	23
2067	Structural and dynamical heterogeneity of water trapped inside Na ⁺ -pumping KR2 rhodopsin in the dark state. <i>Journal of Chemical Physics</i> , 2021, 154, 215101.	1.2	2
2068	Binding of Ca ²⁺ -independent C2 domains to lipid membranes: A multi-scale molecular dynamics study. <i>Structure</i> , 2021, 29, 1200-1213.e2.	1.6	19
2069	Prediction of essential binding domains for the endocannabinoid N-arachidonylethanolamine (AEA) in the brain cannabinoid CB1 receptor. <i>PLoS ONE</i> , 2021, 16, e0229879.	1.1	1
2070	Mechanism of Guanosine Triphosphate Hydrolysis by the Visual Proteins Arl3-RP2: Free Energy Reaction Profiles Computed with Ab Initio Type QM/MM Potentials. <i>Molecules</i> , 2021, 26, 3998.	1.7	7

#	ARTICLE	IF	CITATIONS
2071	Landscape-Based Mutational Sensitivity Cartography and Network Community Analysis of the SARS-CoV-2 Spike Protein Structures: Quantifying Functional Effects of the Circulating D614G Variant. ACS Omega, 2021, 6, 16216-16233.	1.6	10
2072	Key computational findings reveal proton transfer as driving the functional cycle in the phosphate transporter PiPT. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	10
2073	Identification of FDA approved drugs against SARS-CoV-2 RNA dependent RNA polymerase (RdRp) and 3-chymotrypsin-like protease (3CLpro), drug repurposing approach. Biomedicine and Pharmacotherapy, 2021, 138, 111544.	2.5	44
2074	Cryo-EM structure of the photosynthetic RC-LH1-PufX supercomplex at 2.8-Å... resolution. Science Advances, 2021, 7, .	4.7	29
2075	Fast bilayer-micelle fusion mediated by hydrophobic dipeptides. Biophysical Journal, 2021, 120, 2330-2342.	0.2	4
2076	Validating the CHARMM36m protein force field with LJ-PME reveals altered hydrogen bonding dynamics under elevated pressures. Communications Chemistry, 2021, 4, .	2.0	5
2078	Soluble State of Villin Headpiece Protein as a Tool in the Assessment of MD Force Fields. Journal of Physical Chemistry B, 2021, 125, 6897-6911.	1.2	4
2079	The Role of Conserved Residues in the DEDDh Motif: the Proton-Transfer Mechanism of HIV-1 RNase H. ACS Catalysis, 2021, 11, 7915-7927.	5.5	11
2080	Mechanism of Vitamin D Receptor Ligand-Binding Domain Regulation Studied by gREST Simulations. Journal of Chemical Information and Modeling, 2021, 61, 3625-3637.	2.5	3
2081	Optimal Protein Sequence Design Mitigates Mechanical Failure in Silk β -Sheet Nanocrystals. ACS Biomaterials Science and Engineering, 2021, 7, 3156-3165.	2.6	4
2083	Free energy landscape of RNA binding dynamics in start codon recognition by eukaryotic ribosomal pre-initiation complex. PLoS Computational Biology, 2021, 17, e1009068.	1.5	5
2084	Combinatorial phosphorylation modulates the structure and function of the G protein β subunit in yeast. Science Signaling, 2021, 14, .	1.6	4
2086	Activation mechanism of <i>Drosophila</i> cryptochrome through an allosteric switch. Science Advances, 2021, 7, .	4.7	14
2087	Dynamic Profiling of Binding and Allosteric Propensities of the SARS-CoV-2 Spike Protein with Different Classes of Antibodies: Mutational and Perturbation-Based Scanning Reveals the Allosteric Duality of Functionally Adaptable Hotspots. Journal of Chemical Theory and Computation, 2021, 17, 4578-4598.	2.3	39
2088	Elucidating Axonal Injuries Through Molecular Modelling of Myelin Sheaths and Nodes of Ranvier. Frontiers in Molecular Biosciences, 2021, 8, 669897.	1.6	5
2089	<i>In Silico</i> Repositioning of Dopamine Modulators with Possible Application to Schizophrenia: Pharmacophore Mapping, Molecular Docking and Molecular Dynamics Analysis. ACS Omega, 2021, 6, 14748-14764.	1.6	2
2090	Pearling and helical nanostructures of model protocell membranes. Nano Research, 2022, 15, 659.	5.8	2
2091	Sphingomonas sp. KT-1 PahZ2 Structure Reveals a Role for Conformational Dynamics in Peptide Bond Hydrolysis. Journal of Physical Chemistry B, 2021, 125, 5722-5739.	1.2	1

#	ARTICLE	IF	CITATIONS
2092	Generalizing the Discrete Gibbs Sampler-Based $\hat{\mu}$ -Dynamics Approach for Multisite Sampling of Many Ligands. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3895-3907.	2.3	7
2093	Finding Druggable Sites in Proteins Using TACTICS. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2897-2910.	2.5	13
2094	Q-Force: Quantum Mechanically Augmented Molecular Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4946-4960.	2.3	21
2095	Anharmonic Vibrational Calculations Based on Group-Localized Coordinates: Applications to Internal Water Molecules in Bacteriorhodopsin. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5007-5020.	2.3	8
2096	In silico investigation of potential small molecule inhibitors of the SARS-CoV-2 nsp10-nsp16 methyltransferase complex. <i>Chemical Physics Letters</i> , 2021, 774, 138618.	1.2	9
2097	Bacterial Quorum Sensing Signals Promote Large-Scale Remodeling of Lipid Membranes. <i>Langmuir</i> , 2021, 37, 9120-9136.	1.6	10
2098	Cryo-EM structure and dynamics of the green-light absorbing proteorhodopsin. <i>Nature Communications</i> , 2021, 12, 4107.	5.8	15
2099	Irradiation-driven molecular dynamics: a review. <i>European Physical Journal D</i> , 2021, 75, 1.	0.6	6
2101	Anisotropy in mechanical unfolding of protein upon partner-assisted pulling and handle-assisted pulling. <i>Communications Biology</i> , 2021, 4, 925.	2.0	6
2102	Deactivation blocks proton pathways in the mitochondrial complex I. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	21
2103	Size-Selective VAILase Proteolysis Provides Dynamic Insights into Protein Structures. <i>Analytical Chemistry</i> , 2021, 93, 10653-10660.	3.2	1
2104	Homo-oligomerization of the human adenosine A2A receptor is driven by the intrinsically disordered C-terminus. <i>ELife</i> , 2021, 10, .	2.8	8
2105	In-vitro, in-vivo, and in-silico assessment of radical scavenging and cytotoxic activities of <i>Oliveria decumbens</i> essential oil and its main components. <i>Scientific Reports</i> , 2021, 11, 14281.	1.6	14
2108	Maintenance of complex I and its supercomplexes by NDUF-11 is essential for mitochondrial structure, function and health. <i>Journal of Cell Science</i> , 2021, 134, .	1.2	17
2109	Differential Reversible and Irreversible Interactions between Benzbromarone and Human Cytochrome P450s 3A4 and 3A5. <i>Molecular Pharmacology</i> , 2021, 100, 224-236.	1.0	8
2110	Exploring the potential of novel phenolic compounds as potential therapeutic candidates against SARS-CoV-2, using quantum chemistry, molecular docking and dynamic studies. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2021, 43, 128079.	1.0	29
2111	Molecular Modeling Reveals the Mechanism of Ran-RanGAP-Catalyzed Guanosine Triphosphate Hydrolysis without an Arginine Finger. <i>ACS Catalysis</i> , 2021, 11, 8985-8998.	5.5	10
2112	Initial Stages of Spontaneous Binding of Folate-Based Vectors to Folate Receptor- β Observed by Unbiased Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7598-7612.	1.2	5

#	ARTICLE	IF	CITATIONS
2114	Nifuroxazide as JAK2 inhibitor: A binding mode proposal and Hel cell proliferation assay. <i>European Journal of Pharmaceutical Sciences</i> , 2021, 162, 105822.	1.9	3
2115	A novel variant fibrinogen, A1±E11del, demonstrating the importance of A1±E11 residue in thrombin binding. <i>International Journal of Hematology</i> , 2021, 114, 591-598.	0.7	0
2116	Cysteine cross-linking in native membranes establishes the transmembrane architecture of Ire1. <i>Journal of Cell Biology</i> , 2021, 220, .	2.3	8
2117	A general mechanism of KCNE1 modulation of KCNQ1 channels involving non-canonical VSD-PD coupling. <i>Communications Biology</i> , 2021, 4, 887.	2.0	4
2118	Intramolecular interactions play key role in stabilization of pHLIP at acidic conditions. <i>Journal of Computational Chemistry</i> , 2021, 42, 1809-1816.	1.5	1
2119	Delineating the Ligandâ€“Receptor Interactions That Lead to Biased Signaling at the Î¼-Opioid Receptor. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3696-3707.	2.5	14
2120	Water accelerates the hydrogen-bond dynamics and abates heterogeneity in deep eutectic solvent based on acetamide and lithium perchlorate. <i>Journal of Chemical Physics</i> , 2021, 155, 024505.	1.2	8
2121	Exploring the Tunability and Dynamic Properties of MarR-PmarO Sensor System in <i>Escherichia coli</i> . <i>ACS Synthetic Biology</i> , 2021, 10, 2076-2086.	1.9	9
2122	A theoretical approach for the acylation/deacylation mechanisms of avibactam in the reversible inhibition of KPC-2. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 943-952.	1.3	0
2123	Computational assessment of select antiviral phytochemicals as potential SARS-Cov-2 main protease inhibitors: molecular dynamics guided ensemble docking and extended molecular dynamics. <i>In Silico Pharmacology</i> , 2021, 9, 44.	1.8	15
2124	Exploring Post-activation Conformational Changes in Pigeon Cryptochrome 4. <i>Journal of Physical Chemistry B</i> , 2021, 125, 9652-9659.	1.2	18
2125	Exploring dynamics and network analysis of spike glycoprotein of SARS-COV-2. <i>Biophysical Journal</i> , 2021, 120, 2902-2913.	0.2	22
2126	Antipsychotic clozapine binding to alpha-2-macroglobulin protects interacting partners against oxidation and preserves the anti-proteinase activity of the protein. <i>International Journal of Biological Macromolecules</i> , 2021, 183, 502-512.	3.6	5
2127	Atomistic molecular dynamics study on the influence of high temperatures on the structure of peptide nanomembranes candidates for organic supercapacitor electrode. <i>Journal of Molecular Liquids</i> , 2021, 334, 116126.	2.3	15
2128	The Uncommon Active Site of D-Amino Acid Transaminase from <i>Haliscomenobacter hydrossis</i> : Biochemical and Structural Insights into the New Enzyme. <i>Molecules</i> , 2021, 26, 5053.	1.7	14
2129	Characterization of the structural forces governing the reversibility of the thermal unfolding of the human acidic fibroblast growth factor. <i>Scientific Reports</i> , 2021, 11, 15579.	1.6	5
2130	Cardiolipin-Containing Lipid Membranes Attract the Bacterial Cell Division Protein DivIVA. <i>International Journal of Molecular Sciences</i> , 2021, 22, 8350.	1.8	5
2131	Functional cross-talk between phosphorylation and disease-causing mutations in the cardiac sodium channel Na ^v 1.5. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	15

#	ARTICLE	IF	CITATIONS
2132	Cryo-EM structure of the β_3 -adrenergic receptor reveals the molecular basis of subtype selectivity. <i>Molecular Cell</i> , 2021, 81, 3205-3215.e5.	4.5	21
2133	Calcium Ions Promote Membrane Fusion by Forming Negative-Curvature Inducing Clusters on Specific Anionic Lipids. <i>ACS Nano</i> , 2021, 15, 12880-12887.	7.3	23
2134	Effects of Cardiolipin on the Conformational Dynamics of Membrane-Anchored Bcl-xL. <i>International Journal of Molecular Sciences</i> , 2021, 22, 9388.	1.8	4
2136	Adaptations for Pressure and Temperature in Dihydrofolate Reductases. <i>Microorganisms</i> , 2021, 9, 1706.	1.6	3
2137	Electron Transfer Coupled to Conformational Dynamics in Cell Respiration. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 711436.	1.6	4
2139	PIP2-induced membrane binding of the Vinculin tail competes with its other binding partners. <i>Biophysical Journal</i> , 2021, 120, 4608-4622.	0.2	3
2140	Molecular mechanism of thiamine pyrophosphate import into mitochondria: a molecular simulation study. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 987-1007.	1.3	0
2142	QM/MM Simulations of Protein Crystal Reactivity Guided by MSOX Crystallography: A Copper Nitrite Reductase Case Study. <i>Journal of Physical Chemistry B</i> , 2021, 125, 9102-9114.	1.2	3
2145	Identification and assessment of cardiolipin interactions with <i>E. coli</i> inner membrane proteins. <i>Science Advances</i> , 2021, 7, .	4.7	49
2146	Computational study of non-conductive selectivity filter conformations and C-type inactivation in a voltage-dependent potassium channel. <i>Journal of General Physiology</i> , 2021, 153, .	0.9	14
2147	Effect of protein dimerization on ion conductivity of gramicidin a channel studied using polarizable force field. <i>Chinese Journal of Chemical Physics</i> , 2021, 34, 471-479.	0.6	0
2148	An in-silico analysis reveals 7,7-bializarin as a promising DNA gyrase B inhibitor on Gram-positive and Gram-negative bacteria. <i>Computers in Biology and Medicine</i> , 2021, 135, 104626.	3.9	8
2149	A de novo GRIN1 Variant Associated With Myoclonus and Developmental Delay: From Molecular Mechanism to Rescue Pharmacology. <i>Frontiers in Genetics</i> , 2021, 12, 694312.	1.1	6
2150	The interaction of the severe acute respiratory syndrome coronavirus 2 spike protein with drug-inhibited angiotensin converting enzyme 2 studied by molecular dynamics simulation. <i>Journal of Hypertension</i> , 2021, 39, 1705-1716.	0.3	8
2151	Deciphering ion transport and ATPase coupling in the intersubunit tunnel of KdpFABC. <i>Nature Communications</i> , 2021, 12, 5098.	5.8	10
2152	Cryo-EM structure of the human MT1 α -Gi signaling complex. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 694-701.	3.6	31
2156	Inter-pulse delay optimization for dynamical decoupling pulse sequences with up to six refocusing pulses. <i>European Physical Journal Plus</i> , 2021, 136, 1.	1.2	1
2157	Lysine Deacetylase Substrate Selectivity: A Dynamic Ionic Interaction Specific to KDAC8. <i>Biochemistry</i> , 2021, 60, 2524-2536.	1.2	6

#	ARTICLE	IF	CITATIONS
2158	N501Y mutation of spike protein in SARS-CoV-2 strengthens its binding to receptor ACE2. <i>ELife</i> , 2021, 10, .	2.8	262
2159	Phenothiazines alter plasma membrane properties and sensitize cancer cells to injury by inhibiting annexin-mediated repair. <i>Journal of Biological Chemistry</i> , 2021, 297, 101012.	1.6	16
2160	Is Disrupted Nucleotide-Substrate Cooperativity a Common Trait for Cushing's Syndrome Driving Mutations of Protein Kinase A?. <i>Journal of Molecular Biology</i> , 2021, 433, 167123.	2.0	8
2161	The cryo-EM structure of the bd oxidase from <i>M. tuberculosis</i> reveals a unique structural framework and enables rational drug design to combat TB. <i>Nature Communications</i> , 2021, 12, 5236.	5.8	29
2162	Cryo-EM structure of the cetacean morbillivirus nucleoprotein-RNA complex. <i>Journal of Structural Biology</i> , 2021, 213, 107750.	1.3	12
2163	Using Constrained Density Functional Theory to Track Proton Transfers and to Sample Their Associated Free Energy Surface. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5759-5765.	2.3	9
2164	<i>In silico</i> and <i>in vitro</i> assays reveal potential inhibitors against 3CL ^{pro} main protease of SARS-CoV-2. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 12800-12811.	2.0	2
2165	Spontaneous transmembrane pore formation by short-chain synthetic peptide. <i>Biophysical Journal</i> , 2021, 120, 4557-4574.	0.2	6
2166	Topology Automated Force-Field Interactions (TAFFI): A Framework for Developing Transferable Force Fields. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5013-5027.	2.5	11
2167	Structural and functional interactions between the Ca ²⁺ -ATP-, and caffeine-binding sites of skeletal muscle ryanodine receptor (RyR1). <i>Journal of Biological Chemistry</i> , 2021, 297, 101040.	1.6	13
2168	Identifying key determinants and dynamics of SARS-CoV-2/ACE2 tight interaction. <i>PLoS ONE</i> , 2021, 16, e0257905.	1.1	6
2169	Effects of Micellization Behavior on the Interfacial Adsorption in Binary Anionic/Nonionic Surfactant Systems: A Molecular Simulation Study. <i>Langmuir</i> , 2021, 37, 11835-11843.	1.6	6
2170	Dissecting the Role of N-Glycan at N413 in Toll-like Receptor 3 via Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 5258-5266.	2.5	2
2171	TD-DFT absorption spectrum of (poly)threonine in water: A study combining molecular dynamics and quantum mechanics calculations. <i>Chemical Physics Letters</i> , 2021, 779, 138876.	1.2	4
2172	Effect of the Force Field on Molecular Dynamics Simulations of the Multidrug Efflux Protein P-Glycoprotein. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6491-6508.	2.3	17
2173	Molecular determinants of pro-arrhythmia proclivity of d- and l-sotalol via a multi-scale modeling pipeline. <i>Journal of Molecular and Cellular Cardiology</i> , 2021, 158, 163-177.	0.9	10
2174	The SARS-CoV-2 spike protein is vulnerable to moderate electric fields. <i>Nature Communications</i> , 2021, 12, 5407.	5.8	26
2175	Toward Convergence in Free Energy Calculations for Protein Conformational Changes: A Case Study on the Thin Gate of Mhp1 Transporter. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6583-6596.	2.3	3

#	ARTICLE	IF	CITATIONS
2176	Force Field Effects in Simulations of Flexible Peptides with Varying Polyproline II Propensity. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6634-6646.	2.3	24
2177	Computational modeling and experimental validation of the EPI-X4/CXCR4 complex allows rational design of small peptide antagonists. <i>Communications Biology</i> , 2021, 4, 1113.	2.0	20
2178	Peptide inhibitors against SARS-CoV-2 2â€²-O-methyltransferase involved in RNA capping: A computational approach. <i>Biochemistry and Biophysics Reports</i> , 2021, 27, 101069.	0.7	5
2179	Solution structures of human myeloma IgG3 antibody reveal extended Fab and Fc regions relative to the other IgG subclasses. <i>Journal of Biological Chemistry</i> , 2021, 297, 100995.	1.6	8
2180	A second S4 movement opens hyperpolarization-activated HCN channels. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	9
2181	A comparison of three DFT exchangeâ€“correlation functionals and two basis sets for the prediction of the conformation distribution of hydrated polyglycine. <i>Journal of Chemical Physics</i> , 2021, 155, 094104.	1.2	6
2182	The E₂ state of FeMoco: Hydride Formation versus Fe Reduction and a Mechanism for H₂ Evolution. <i>Chemistry - A European Journal</i> , 2021, 27, 16788-16800.	1.7	22
2184	Lpp positions peptidoglycan at the AcrA-TolC interface in the AcrAB-TolC multidrug efflux pump. <i>Biophysical Journal</i> , 2021, 120, 3973-3982.	0.2	13
2186	Open-state structure and pore gating mechanism of the cardiac sodium channel. <i>Cell</i> , 2021, 184, 5151-5162.e11.	13.5	56
2187	Unlocking the secret of lignin-enzyme interactions: Recent advances in developing state-of-the-art analytical techniques. <i>Biotechnology Advances</i> , 2022, 54, 107830.	6.0	44
2188	Atomistic Simulations and In Silico Mutational Profiling of Protein Stability and Binding in the SARS-CoV-2 Spike Protein Complexes with Nanobodies: Molecular Determinants of Mutational Escape Mechanisms. <i>ACS Omega</i> , 2021, 6, 26354-26371.	1.6	11
2189	Effect of Strain Rate on Single Tau, Dimerized Tau and Tau-Microtubule Interface: A Molecular Dynamics Simulation Study. <i>Biomolecules</i> , 2021, 11, 1308.	1.8	3
2190	Accurate and Transferable Reactive Molecular Dynamics Models from Constrained Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2021, 125, 10471-10480.	1.2	11
2191	Corrections in the CHARMM36 Parametrization of Chloride Interactions with Proteins, Lipids, and Alkali Cations, and Extension to Other Halide Anions. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6240-6261.	2.3	7
2192	Cryo-EM structure of the sodium-driven chloride/bicarbonate exchanger NDCBE. <i>Nature Communications</i> , 2021, 12, 5690.	5.8	24
2193	Mechanical couplings of protein backbone and side chains exhibit scale-free network properties and specific hotspots for function. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 5309-5320.	1.9	5
2194	Modification of a Single Atom Affects the Physical Properties of Double Fluorinated Fmoc-Phe Derivatives. <i>International Journal of Molecular Sciences</i> , 2021, 22, 9634.	1.8	9
2195	Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of PHF6 Peptide of Tau Protein. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6458-6471.	2.3	23

#	ARTICLE	IF	CITATIONS
2196	Influence of Lipid Bilayer on the GPCR Structure: Comparison of All-Atom Lipid Force Fields. Bulletin of the Chemical Society of Japan, 2021, 94, 2569-2574.	2.0	9
2197	Integrin-based mechanosensing through conformational deformation. Biophysical Journal, 2021, 120, 4349-4359.	0.2	10
2198	Detection of Amyloid- β Fibrils Using Track-Etched Nanopores: Effect of Geometry and Crowding. ACS Sensors, 2021, 6, 3733-3743.	4.0	20
2199	Allosteric Control of Structural Mimicry and Mutational Escape in the SARS-CoV-2 Spike Protein Complexes with the ACE2 Decoys and Miniprotein Inhibitors: A Network-Based Approach for Mutational Profiling of Binding and Signaling. Journal of Chemical Information and Modeling, 2021, 61, 5172-5191.	2.5	26
2202	O to bR transition in bacteriorhodopsin occurs through a proton hole mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	5
2203	Atypical kinetics of cytochrome P450 2J2: Epoxidation of arachidonic acid and reversible inhibition by xenobiotic inhibitors. European Journal of Pharmaceutical Sciences, 2021, 164, 105889.	1.9	9
2204	Binding Mechanism of Neutralizing Nanobodies Targeting SARS-CoV-2 Spike Glycoprotein. Journal of Chemical Information and Modeling, 2021, 61, 5152-5160.	2.5	11
2205	Covalent inhibition of hAChE by organophosphates causes homodimer dissociation through long-range allosteric effects. Journal of Biological Chemistry, 2021, 297, 101007.	1.6	8
2206	Probe Confined Dynamic Mapping for G Protein-Coupled Receptor Allosteric Site Prediction. ACS Central Science, 2021, 7, 1847-1862.	5.3	15
2207	Bacterial Luciferases from <i>Vibrio harveyi</i> and <i>Photobacterium leiognathi</i> Demonstrate Different Conformational Stability as Detected by Time-Resolved Fluorescence Spectroscopy. International Journal of Molecular Sciences, 2021, 22, 10449.	1.8	3
2208	Advanced Sampling Methods for Multiscale Simulation of Disordered Proteins and Dynamic Interactions. Biomolecules, 2021, 11, 1416.	1.8	17
2212	$\hat{\alpha}$ -tocopherol, a slow-binding inhibitor of acetylcholinesterase. Chemico-Biological Interactions, 2021, 348, 109646.	1.7	4
2213	Hydroxylic, sulfur-containing and amidic amino acids in water solution: Atomic charges parameters for computational modeling using molecular dynamics simulation and DFT calculations. Journal of Molecular Liquids, 2021, 339, 116815.	2.3	6
2215	Laminar peptide structure: Energetic and structural evaluation using molecular dynamics. Journal of Molecular Liquids, 2021, 341, 117261.	2.3	4
2216	Novel molecular insight into the discrepant distributions for ionic surfactants in light oil/water and heavy oil/water systems. Fuel, 2021, 304, 121460.	3.4	11
2217	Interplay between human islet amyloid polypeptide aggregates and micro-heterogeneous membranes. Biochimica Et Biophysica Acta - Biomembranes, 2021, 1863, 183691.	1.4	3
2218	Ripple-like instability in the simulated gel phase of finite size phosphocholine bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2021, 1863, 183714.	1.4	6
2219	One-step preparation of the engineered titanium implant by rationally designed linear fusion peptides with spacer-dependent antimicrobial, anti-inflammatory and osteogenic activities. Chemical Engineering Journal, 2021, 424, 130380.	6.6	8

#	ARTICLE	IF	CITATIONS
2220	Protein simulation in supercritical CO ₂ : The challenge of force field. <i>Journal of Molecular Liquids</i> , 2021, 343, 117662.	2.3	6
2221	Multi-Spectroscopic, thermodynamic and molecular dynamic simulation studies for investigation of interaction of dapagliflozin with bovine serum albumin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 264, 120298.	2.0	37
2222	Constraints on error rate revealed by computational study of Gâ€U tautomerization in translation. <i>Nucleic Acids Research</i> , 2021, 49, 11823-11833.	6.5	3
2223	Computational Study of Helical and Helix-Hinge-Helix Conformations of an Anti-Microbial Peptide in Solution by Molecular Dynamics and Vibrational Analysis. <i>Journal of Physical Chemistry B</i> , 2021, 125, 703-721.	1.2	5
2224	Valproik Asit ile CYP2C9 MutantlarÄ± F114L ve I207T MolekÃ¼ler EtkileÅŸimlerinin Ä±zlenmesi iÅŸin MolekÃ¼ler Dinamik ve MM-PBSA Ä±lÄ±ymalarÄ±. <i>Journal of Natural and Applied Sciences</i> , 0, , .	0.1	0
2225	Discovery of beta-lactamase CMY-10 inhibitors for combination therapy against multi-drug resistant Enterobacteriaceae. <i>PLoS ONE</i> , 2021, 16, e0244967.	1.1	19
2226	Dynamic Preference for NADP/H Cofactor Binding/Release in E. coli YqhD Oxidoreductase. <i>Molecules</i> , 2021, 26, 270.	1.7	3
2227	Identification of multiple substrate binding sites in SLC4 transporters in the outward-facing conformation: Insights into the transport mechanism. <i>Journal of Biological Chemistry</i> , 2021, 296, 100724.	1.6	15
2228	Mechanistic Basis of OXA-48-like Î²-Lactamasesâ€™ Hydrolysis of Carbapenems. <i>ACS Infectious Diseases</i> , 2021, 7, 445-460.	1.8	18
2230	Weakening of interaction networks with aging in tip-link protein induces hearing loss. <i>Biochemical Journal</i> , 2021, 478, 121-134.	1.7	7
2232	Origin of the Surprising Mechanical Stability of Kinesinâ€™s Neck Coiled Coil. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1017-1029.	2.3	1
2233	Active participation of membrane lipids in inhibition of multidrug transporter P-glycoprotein. <i>Chemical Science</i> , 2021, 12, 6293-6306.	3.7	20
2234	Mechanism of C-type inactivation in the hERG potassium channel. <i>Science Advances</i> , 2021, 7, .	4.7	26
2235	Preparing and Analyzing Polarizable Molecular Dynamics Simulations with the Classical Drude Oscillator Model. <i>Methods in Molecular Biology</i> , 2021, 2315, 219-240.	0.4	2
2236	Crowding-induced opening of the mechanosensitive Piezo1 channel in silico. <i>Communications Biology</i> , 2021, 4, 84.	2.0	35
2237	Computational simulations reveal the binding dynamics between human ACE2 and the receptor binding domain of SARSâ€CoVâ€2 spike protein. <i>Quantitative Biology</i> , 2021, 9, 61-72.	0.3	15
2238	Introducing P ep McConst â€™A userâ€™friendly peptide modeler for biophysical applications. <i>Journal of Computational Chemistry</i> , 2021, 42, 572-580.	1.5	8
2239	Molecular perspective on charge-tunable adsorption of volatile organic compounds on carbon nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2972-2980.	1.3	14

#	ARTICLE	IF	CITATIONS
2240	Study of Candesartan Cilexetil: 2-Hydroxypropyl- β -Cyclodextrin : A Computational Approach Using Steered Simulations. <i>Methods in Molecular Biology</i> , 2021, 2207, 45-70.	0.4	1
2241	Site Identification by Ligand Competitive Saturation (SILCS) Simulations for Fragment-Based Drug Design. <i>Methods in Molecular Biology</i> , 2015, 1289, 75-87.	0.4	37
2242	Atomistic Force Fields for Proteins. <i>Methods in Molecular Biology</i> , 2019, 2022, 3-19.	0.4	14
2243	Proteinâ€™Ligand Binding Free Energy Calculations with FEP+. <i>Methods in Molecular Biology</i> , 2019, 2022, 201-232.	0.4	43
2244	Molecular Dynamics Simulation of Proteins. <i>Methods in Molecular Biology</i> , 2020, 2073, 311-327.	0.4	47
2245	Polarizable Force Fields for Proteins. , 2014, , 91-134.		10
2246	Molecular Mechanics: Principles, History, and Current Status. , 2015, , 1-48.		4
2247	Distance-Based Metrics for Comparing Conformational Ensembles of Intrinsically Disordered Proteins. <i>Biophysical Journal</i> , 2020, 118, 2952-2965.	0.2	17
2248	Dynamics-Driven Allostery Underlies Ca ²⁺ -Mediated Release of SERCA Inhibition by Phospholamban. <i>Biophysical Journal</i> , 2020, 119, 1917-1926.	0.2	10
2249	Multiscale Simulations Examining Glycan Shield Effects on Drug Binding to Influenza Neuraminidase. <i>Biophysical Journal</i> , 2020, 119, 2275-2289.	0.2	13
2250	Elucidating NH ₂ -I3V3A3G3K3-COOH and NH ₂ -K3G3A3V3I3-COOH polypeptide membranes: A classical molecular dynamics study. <i>Journal of Molecular Liquids</i> , 2019, 279, 740-749.	2.3	20
2251	The effect of water/ethanol solvent mixtures on interactions of an antibody selective for wild-type alpha-1-antitrypsin in complex with its antigen. <i>Journal of Molecular Liquids</i> , 2020, 312, 113437.	2.3	4
2252	The dynamics of β -secretase and its substrates. <i>Seminars in Cell and Developmental Biology</i> , 2020, 105, 86-101.	2.3	19
2253	Infectivity of Dengue Virus Serotypes 1 and 2 Is Correlated with E-Protein Intrinsic Dynamics but Not to Envelope Conformations. <i>Structure</i> , 2019, 27, 618-630.e4.	1.6	23
2254	Mechanism of Inward Proton Transport in an Antarctic Microbial Rhodopsin. <i>Journal of Physical Chemistry B</i> , 2020, 124, 4851-4872.	1.2	29
2255	Exploring the Thermodynamics of 7-Amino Actinomycin D-Induced Single-Stranded DNA Hairpin by Spectroscopic Techniques and Computational Simulations. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10007-10013.	1.2	2
2256	How Pure and Hydrated Reline Deep Eutectic Solvents Affect the Conformation and Stability of Lysozyme: Insights from Atomistic Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11919-11927.	1.2	28
2257	Characterizing the structural ensemble of β -secretase using a multiscale molecular dynamics approach. <i>Chemical Science</i> , 2017, 8, 5576-5584.	3.7	55

#	ARTICLE	IF	CITATIONS
2258	Sunitinib inhibits RNase L by destabilizing its active dimer conformation. <i>Biochemical Journal</i> , 2020, 477, 3387-3399.	1.7	10
2259	Microscopic insight into thermodynamics of conformational changes of SAP-SLAM complex in signal transduction cascade. <i>Journal of Chemical Physics</i> , 2017, 146, 165103.	1.2	4
2260	Functional insights into the mode of DNA and ligand binding of the TetR family regulator TylP from <i>Streptomyces fradiae</i> . <i>Journal of Biological Chemistry</i> , 2017, 292, 15301-15311.	1.6	12
2261	The scrutinised DFT and MD studies on the adsorption of D-penicillamine drug on Fe_2O_3 nanoparticle as a highly efficient carrier. <i>Molecular Simulation</i> , 2020, 46, 408-418.	0.9	1
2262	Sensing of nutrients by CPT1C controls SAC1 activity to regulate AMPA receptor trafficking. <i>Journal of Cell Biology</i> , 2020, 219, .	2.3	18
2263	The basic residues in the Orai1 channel inner pore promote opening of the outer hydrophobic gate. <i>Journal of General Physiology</i> , 2020, 152, .	0.9	21
2264	A novel voltage-clamp/dye uptake assay reveals saturable transport of molecules through CALHM1 and connexin channels. <i>Journal of General Physiology</i> , 2020, 152, .	0.9	8
2265	Transmembrane motions of PglB induced by LLO are coupled with EL5 loop conformational changes necessary for OST activity. <i>Glycobiology</i> , 2017, 27, 734-742.	1.3	6
2326	Atomistic modelling of scattering data in the Collaborative Computational Project for Small Angle Scattering (CCP-SAS). <i>Journal of Applied Crystallography</i> , 2016, 49, 1861-1875.	1.9	67
2327	Atom interaction propensities of oxygenated chemical functions in crystal packings. <i>IUCrJ</i> , 2017, 4, 158-174.	1.0	23
2328	Elucidation of DNA Repair Function of PfBlm and Potentiation of Artemisinin Action by a Small-Molecule Inhibitor of RecQ Helicase. <i>MSphere</i> , 2020, 5, .	1.3	5
2329	The Effect of Osmolytes on the Bioluminescent Reaction of Bacteria: Structural and Dynamic Properties. <i>Biophysics (Russian Federation)</i> , 2020, 65, 966-971.	0.2	4
2330	Hybrid Spectral/Subspace Clustering of Molecular Dynamics Simulations. , 2018, , .		2
2331	Oxidative hotspots on actin promote skeletal muscle weakness in rheumatoid arthritis. <i>JCI Insight</i> , 2019, 4, .	2.3	23
2332	Commensal bacteria stimulate antitumor responses via T cell cross-reactivity. <i>JCI Insight</i> , 2020, 5, .	2.3	95
2333	A voltage-dependent fluorescent indicator for optogenetic applications, archaerhodopsin-3: Structure and optical properties from in silico modeling. <i>F1000Research</i> , 2017, 6, 33.	0.8	8
2334	A voltage-dependent fluorescent indicator for optogenetic applications, archaerhodopsin-3: Structure and optical properties from in silico modeling. <i>F1000Research</i> , 2017, 6, 33.	0.8	6
2335	The Molecular Basis of Polyunsaturated Fatty Acid Interactions with the Shaker Voltage-Gated Potassium Channel. <i>PLoS Computational Biology</i> , 2016, 12, e1004704.	1.5	47

#	ARTICLE	IF	CITATIONS
2336	Dynamic Cholesterol-Conditioned Dimerization of the G Protein Coupled Chemokine Receptor Type 4. <i>PLoS Computational Biology</i> , 2016, 12, e1005169.	1.5	75
2337	Is the Conformational Ensemble of Alzheimer's A β 210-40 Peptide Force Field Dependent?. <i>PLoS Computational Biology</i> , 2017, 13, e1005314.	1.5	22
2338	The E2.65A mutation disrupts dynamic binding poses of SB269652 at the dopamine D2 and D3 receptors. <i>PLoS Computational Biology</i> , 2018, 14, e1005948.	1.5	19
2339	Characterization of a Novel BCHE "Silent" Allele: Point Mutation (p.Val204Asp) Causes Loss of Activity and Prolonged Apnea with Suxamethonium. <i>PLoS ONE</i> , 2014, 9, e101552.	1.1	34
2340	Study of the Affinity between the Protein Kinase PKA and Peptide Substrates Derived from Kempptide Using Molecular Dynamics Simulations and MM/GBSA. <i>PLoS ONE</i> , 2014, 9, e109639.	1.1	17
2341	Modeling the Interaction between Quinolate and the Receptor for Advanced Glycation End Products (RAGE): Relevance for Early Neuropathological Processes. <i>PLoS ONE</i> , 2015, 10, e0120221.	1.1	17
2342	Towards Development of Small Molecule Lipid II Inhibitors as Novel Antibiotics. <i>PLoS ONE</i> , 2016, 11, e0164515.	1.1	7
2343	Membrane Assembly and Ion Transport Ability of a Fluorinated Nanopore. <i>PLoS ONE</i> , 2016, 11, e0166587.	1.1	6
2344	Supercomputer Docking. <i>Supercomputing Frontiers and Innovations</i> , 2019, 6, .	0.5	3
2345	Free energy profile of permeation of Entecavir through Hepatitis B virus capsid studied by molecular dynamics calculation. <i>Pure and Applied Chemistry</i> , 2020, 92, 1585-1594.	0.9	3
2346	A computer-based approach for developing linamarase inhibitory agents. <i>ChemistrySelect</i> , 2020, 5, .	0.7	3
2347	Structural basis of Focal Adhesion Kinase activation on lipid membranes. <i>EMBO Journal</i> , 2020, 39, e104743.	3.5	47
2348	Multi-kinase inhibitors can associate with heat shock proteins through their NH2-termini by which they suppress chaperone function. <i>Oncotarget</i> , 2016, 7, 12975-12996.	0.8	44
2349	MRP4/ABCC4 As a New Therapeutic Target: Meta-Analysis to Determine cAMP Binding Sites as a Tool for Drug Design. <i>Current Medicinal Chemistry</i> , 2019, 26, 1270-1307.	1.2	18
2350	Molecular Mechanics. <i>Current Pharmaceutical Design</i> , 2014, 20, 3281-3292.	0.9	87
2351	Shining Light on an mGlu5 Photoswitchable NAM: A Theoretical Perspective. <i>Current Neuropharmacology</i> , 2016, 14, 441-454.	1.4	18
2353	Modeling of the Binding of Peptide Blockers to Voltage-Gated Potassium Channels: Approaches and Evidence. <i>Acta Naturae</i> , 2016, 8, 35-46.	1.7	11
2355	Dynamical Correlations Reveal Allosteric Sites in G Protein-Coupled Receptors. <i>International Journal of Molecular Sciences</i> , 2021, 22, 187.	1.8	6

#	ARTICLE	IF	CITATIONS
2356	Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. <i>Processes</i> , 2021, 9, 71.	1.3	162
2357	Probing $\hat{\mu}/\hat{\nu}^2$ Balances in Modified Amber Force Fields from a Molecular Dynamics Study on a $\hat{\mu}^2/\hat{\nu}^2$ Model Protein (1FSD). <i>Bulletin of the Korean Chemical Society</i> , 2014, 35, 1713-1719.	1.0	3
2358	Structural Change in Transmembrane Region of Syndecan-4 by Mutation. <i>Journal of the Korean Magnetic Resonance Society</i> , 2016, 20, 129-137.	0.1	2
2359	Single molecule FRET reveals pore size and opening mechanism of a mechano-sensitive ion channel. <i>ELife</i> , 2014, 3, e01834.	2.8	116
2360	Structural insights into the mechanism of activation of the TRPV1 channel by a membrane-bound tarantula toxin. <i>ELife</i> , 2016, 5, .	2.8	71
2361	Molecular dynamics-based refinement and validation for sub-5 Å... cryo-electron microscopy maps. <i>ELife</i> , 2016, 5, .	2.8	136
2362	Proton currents constrain structural models of voltage sensor activation. <i>ELife</i> , 2016, 5, .	2.8	32
2363	Atomic mutagenesis in ion channels with engineered stoichiometry. <i>ELife</i> , 2016, 5, .	2.8	23
2364	Biomolecular interactions modulate macromolecular structure and dynamics in atomistic model of a bacterial cytoplasm. <i>ELife</i> , 2016, 5, .	2.8	238
2365	Structure and dynamics underlying elementary ligand binding events in human pacemaking channels. <i>ELife</i> , 2016, 5, .	2.8	42
2366	Helical jackknives control the gates of the double-pore K ⁺ uptake system KtrAB. <i>ELife</i> , 2017, 6, .	2.8	23
2367	Mechanism of activation at the selectivity filter of the KcsA K ⁺ channel. <i>ELife</i> , 2017, 6, .	2.8	43
2368	Model for a novel membrane envelope in a filamentous hyperthermophilic virus. <i>ELife</i> , 2017, 6, .	2.8	37
2369	Structural insight into the activation of a class B G-protein-coupled receptor by peptide hormones in live human cells. <i>ELife</i> , 2017, 6, .	2.8	42
2370	Key steps in unconventional secretion of fibroblast growth factor 2 reconstituted with purified components. <i>ELife</i> , 2017, 6, .	2.8	63
2371	Free-energy simulations reveal molecular mechanism for functional switch of a DNA helicase. <i>ELife</i> , 2018, 7, .	2.8	15
2372	Fish-hunting cone snail venoms are a rich source of minimized ligands of the vertebrate insulin receptor. <i>ELife</i> , 2019, 8, .	2.8	49
2373	ATP-induced asymmetric pre-protein folding as a driver of protein translocation through the Sec machinery. <i>ELife</i> , 2019, 8, .	2.8	32

#	ARTICLE	IF	CITATIONS
2374	Mechanism of completion of peptidyltransferase centre assembly in eukaryotes. <i>ELife</i> , 2019, 8, .	2.8	49
2375	Trans-toxin ion-sensitivity of charybdotoxin-blocked potassium-channels reveals unbinding transitional states. <i>ELife</i> , 2019, 8, .	2.8	8
2376	Molecular mechanisms of human P2X3 receptor channel activation and modulation by divalent cation bound ATP. <i>ELife</i> , 2019, 8, .	2.8	30
2377	Membrane interactions of the globular domain and the hypervariable region of KRAS4b define its unique diffusion behavior. <i>ELife</i> , 2020, 9, .	2.8	23
2378	Large-scale state-dependent membrane remodeling by a transporter protein. <i>ELife</i> , 2019, 8, .	2.8	42
2379	$\hat{\Gamma}^{11-12}$ linker isomerization governs acid-sensing ion channel desensitization and recovery. <i>ELife</i> , 2020, 9, .	2.8	30
2380	Divergent Cl ⁻ and H ⁺ pathways underlie transport coupling and gating in CLC exchangers and channels. <i>ELife</i> , 2020, 9, .	2.8	17
2381	Distinct inactive conformations of the dopamine D2 and D3 receptors correspond to different extents of inverse agonism. <i>ELife</i> , 2020, 9, .	2.8	31
2382	Multi-state recognition pathway of the intrinsically disordered protein kinase inhibitor by protein kinase A. <i>ELife</i> , 2020, 9, .	2.8	16
2383	A two-lane mechanism for selective biological ammonium transport. <i>ELife</i> , 2020, 9, .	2.8	23
2384	Breakage of the oligomeric CaMKII hub by the regulatory segment of the kinase. <i>ELife</i> , 2020, 9, .	2.8	25
2385	Bacterial OTU deubiquitinases regulate substrate ubiquitination upon <i>Legionella</i> infection. <i>ELife</i> , 2020, 9, .	2.8	23
2386	Mechanistic insights into volatile anesthetic modulation of K2P channels. <i>ELife</i> , 2020, 9, .	2.8	10
2387	A sulfur-aromatic gate latch is essential for opening of the Orai1 channel pore. <i>ELife</i> , 2020, 9, .	2.8	13
2388	Allosteric pockets and dynamic residue network hubs of falcipain 2 in mutations including those linked to artemisinin resistance. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 5647-5666.	1.9	13
2389	Regulation of aquaporin-3 water permeability by hyaluronan. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 25706-25711.	1.3	5
2390	QM/MM modeling of class A $\hat{\Gamma}^2$ -lactamases reveals distinct acylation pathways for ampicillin and cefalexin. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 9182-9189.	1.5	7
2391	Biophysical Methods to Investigate Hydration Structures of Proteins. <i>Soft and Biological Matter</i> , 2021, , 25-59.	0.3	0

#	ARTICLE	IF	CITATIONS
2392	Molecular Modeling of the HR2 and Transmembrane Domains of the SARS-CoV-2 S Protein in the Prefusion State. <i>Moscow University Biological Sciences Bulletin</i> , 2021, 76, 130-136.	0.1	0
2393	Computer Modeling of Structures of Reversibly Switchable Fluorescent Proteins with LOV Domains. <i>Crystallography Reports</i> , 2021, 66, 815-818.	0.1	1
2394	A heuristic, computer-driven and top-down approach to identify novel bioactive peptides: A proof-of-principle on angiotensin I converting enzyme inhibitory peptides. <i>Food Research International</i> , 2021, 150, 110753.	2.9	9
2395	Binding Sites and the Mechanism of Action of Propofol and a Photoreactive Analogue in Prokaryotic Voltage-Gated Sodium Channels. <i>ACS Chemical Neuroscience</i> , 2021, 12, 3898-3914.	1.7	3
2396	All-atom molecular dynamics study of hepatitis B virus containing pregenome RNA in solution. <i>Journal of Chemical Physics</i> , 2021, 155, 145101.	1.2	3
2397	Kinetics of Phenol Escape from the Insulin R ₆ Hexamer. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11637-11649.	1.2	5
2398	Two Sides of Quantum-Based Modeling of Enzyme-Catalyzed Reactions: Mechanistic and Electronic Structure Aspects of the Hydrolysis by Glutamate Carboxypeptidase. <i>Molecules</i> , 2021, 26, 6280.	1.7	4
2399	Spotlight onto surfactantâ€“steamâ€“bitumen interfacial behavior via molecular dynamics simulation. <i>Scientific Reports</i> , 2021, 11, 19660.	1.6	26
2400	How to strike a conformational balance in protein force fields for molecular dynamics simulations?. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2022, 12, e1578.	6.2	4
2401	Computational Analysis of Chemical Space of Natural Compounds Interacting with Sulfotransferases. <i>Molecules</i> , 2021, 26, 6360.	1.7	3
2402	PIP2-dependent coupling of voltage sensor and pore domains in Kv7.2 channel. <i>Communications Biology</i> , 2021, 4, 1189.	2.0	7
2403	Transient local secondary structure in the intrinsically disordered C-term of the Albino3 insertase. <i>Biophysical Journal</i> , 2021, 120, 4992-5004.	0.2	2
2404	Structural Ensemble of the Insulin Monomer. <i>Biochemistry</i> , 2021, 60, 3125-3136.	1.2	5
2405	Double Proton Transfer during a Novel Tertiary Î±-Ketol Rearrangement in Ketol-Acid Reductoisomerase: A Water-Mediated, Metal-Catalyzed, Base-Induced Mechanism. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11893-11906.	1.2	2
2406	Molecular dynamics modeling of the <i>Vibrio cholera</i> Na ⁺ -translocating NADH:quinone oxidoreductase NqrBâ€“NqrD subunit interface. <i>Molecular and Cellular Biochemistry</i> , 2022, 477, 153-165.	1.4	1
2407	Development of CHARMM Additive Potential Energy Parameters for Î±-Methyl Amino Acids. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11687-11696.	1.2	0
2408	High-Performance Biomimetic Water Channel: The Constructive Interplay of Interaction Parameters and Hydrophilic Doping Levels. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11566-11581.	1.2	3
2409	Osh6 Revisited: Control of PS Transport by the Concerted Actions of PI4P and Sac1 Phosphatase. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 747601.	1.6	8

#	ARTICLE	IF	CITATIONS
2410	IgG1 conformational behavior: elucidation of the N-glycosylation role via molecular dynamics. Biophysical Journal, 2021, 120, 5355-5370.	0.2	9
2411	Description of Joint Alterations Observed in a Family Carrying p.Asn453Ser COMP Variant: Clinical Phenotypes, In Silico Prediction of Functional Impact on COMP Protein and Stability, and Review of the Literature. Biomolecules, 2021, 11, 1460.	1.8	1
2413	Molecular insights into receptor binding of recent emerging SARS-CoV-2 variants. Nature Communications, 2021, 12, 6103.	5.8	117
2414	DINC-COVID: A webserver for ensemble docking with flexible SARS-CoV-2 proteins. Computers in Biology and Medicine, 2021, 139, 104943.	3.9	8
2416	In Silico Prediction of the Phosphorylation of NS3 as an Essential Mechanism for Dengue Virus Replication and the Antiviral Activity of Quercetin. Biology, 2021, 10, 1067.	1.3	5
2418	Generalizable coordination of large multiscale workflows. , 2021, , .		17
2419	Preferential binding affinity of ions and their effect on structure and dynamics of water near antimicrobial peptide. Journal of Molecular Liquids, 2021, 344, 117789.	2.3	5
2421	A Five-Residue Insertion Between Codons 28 and 29 of the HIV-1 Protease Gene Reduces the Replicative Capacity of the Virus. Open Forum Infectious Diseases, 2015, 2, .	0.4	0
2422	Chapter 2. Molecular Dynamics Simulations: Principles and Applications for the Study of Membrane Proteins. RSC Theoretical and Computational Chemistry Series, 2016, , 19-58.	0.7	0
2423	Determining the Aggregation Prone Structure of hIAPP. Springer Theses, 2016, , 63-86.	0.0	0
2424	MD Simulations of P-Type ATPases in a Lipid Bilayer System. Methods in Molecular Biology, 2016, 1377, 459-492.	0.4	0
2435	Infectivity of Dengue Virus Serotypes 1 and 2 is Correlated to E Protein Intrinsic Dynamics But Not to Envelope Conformations. SSRN Electronic Journal, 0, , .	0.4	0
2436	Molecular Dynamics-Decorated Finite Element Method (MDeFEM): Application to the Gating Mechanism of Mechanosensitive Channels. , 2018, , 1-52.		0
2449	Molecular Mechanics. , 0, , 279-300.		0
2459	Mesoscale Computational Modeling of Protein-Membrane Interactions Based on Continuum Mean-Field Theory. Methods in Molecular Biology, 2019, 1860, 15-31.	0.4	1
2466	The Molecular Dynamics Simulation of a Multi-domain Outer Membrane Protein A (OmpA) from Shigella flexneri in POPE Lipid Bilayer. , 2019, , 71-83.		0
2467	<i>In silico</i> investigation of the interaction between the voltage-gated potassium channel Kv4.3 and its auxiliary protein KChIP1. Physical Chemistry Chemical Physics, 2019, 21, 25290-25301.	1.3	2
2513	Paracellular Gatekeeping: What Does It Take for an Ion to Pass Through a Tight Junction Pore?. Langmuir, 2020, 36, 6757-6764.	1.6	10

#	ARTICLE	IF	CITATIONS
2528	Oscillation of S5 helix under different temperatures in determination of the open probability of TRPV1 channel. <i>Chinese Physics B</i> , 2020, 29, 098701.	0.7	3
2531	Bayesian Estimation of the Hydroxyl Radical Diffusion Coefficient at Low Temperature and High Pressure from Atomistic Molecular Dynamics. <i>Journal of Chemical Physics</i> , 2021, 155, 194504.	1.2	1
2532	Structural basis for high selectivity of a rice silicon channel Lsi1. <i>Nature Communications</i> , 2021, 12, 6236.	5.8	34
2533	Inside and Out of the Pore: Comparing Interactions and Molecular Dynamics of Influenza A M2 Viroporin Complexes in Standard Lipid Bilayers. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5550-5568.	2.5	5
2534	Reversible Self-Association in Lactate Dehydrogenase during Freeze-Thaw in Buffered Solutions Using Neutron Scattering. <i>Molecular Pharmaceutics</i> , 2021, 18, 4459-4474.	2.3	10
2535	A missense mutation converts the Na ⁺ ,K ⁺ -ATPase into an ion channel and causes therapy-resistant epilepsy. <i>Journal of Biological Chemistry</i> , 2021, 297, 101355.	1.6	9
2536	The Q61H mutation decouples KRAS from upstream regulation and renders cancer cells resistant to SHP2 inhibitors. <i>Nature Communications</i> , 2021, 12, 6274.	5.8	22
2537	Experimental and Simulation Study of the Solvent Effects on the Intrinsic Properties of Spherical Lignin Nanoparticles. <i>Journal of Physical Chemistry B</i> , 2021, 125, 12315-12328.	1.2	21
2538	The Impact of Mutation L138F/L210F on the Orai Channel: A Molecular Dynamics Simulation Study. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 755247.	1.6	4
2539	Development and Testing of Force Field Parameters for Phenylalanine and Tyrosine Derivatives. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 608931.	1.6	2
2541	Design of novel granulopoietic proteins by topological resc scaffolding. <i>PLoS Biology</i> , 2020, 18, e3000919.	2.6	8
2548	Mechanism of Naphthoquinone Selectivity of Thymidylate Synthase ThyX. <i>Biophysical Journal</i> , 2020, 119, 2508-2516.	0.2	2
2549	Developing Kinase Inhibitors Using Computer-Aided Drug Design Approaches. , 2020, , 81-108.		0
2550	Molecular recognition in the product site of cellobiohydrolase Cel7A regulates processive step length. <i>Biochemical Journal</i> , 2020, 477, 99-110.	1.7	4
2551	Molecular Dynamics Flexible Fitting: All You Want to Know About Resolution Exchange. <i>Methods in Molecular Biology</i> , 2020, 2165, 301-315.	0.4	5
2561	Maturation of siRNA by strand separation: Steered molecular dynamics study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 13682-13692.	2.0	2
2562	Thermostabilization mechanisms in thermophilic versus mesophilic three-helix bundle proteins. <i>Journal of Computational Chemistry</i> , 2022, 43, 197-205.	1.5	3
2563	Long-lived room temperature phosphorescent system: Phenanthrene- β -cyclodextrin-tert-butylbenzene. Spectra and structure computer simulations. <i>Journal of Luminescence</i> , 2021, 242, 118581.	1.5	1

#	ARTICLE	IF	CITATIONS
2564	Extended antibody-framework-to-antigen distance observed exclusively with broad HIV-1-neutralizing antibodies recognizing glycan-dense surfaces. <i>Nature Communications</i> , 2021, 12, 6470.	5.8	3
2565	A target fishing study to spot possible biological targets of fusaric acid: Inhibition of protein kinase-A and insights on the underpinning mechanisms. <i>Food and Chemical Toxicology</i> , 2022, 159, 112663.	1.8	6
2566	Kinetics and Mechanism of Fentanyl Dissociation from the μ -Opioid Receptor. <i>Jacs Au</i> , 2021, 1, 2208-2215.	3.6	21
2568	Novel Insights into the Self-assembly Behaviors of Cationic Surfactant and Bivalent Acid: Effects of Group Positions in Bivalent Acid. <i>Journal of Molecular Liquids</i> , 2021, , 118012.	2.3	0
2569	Rational prioritization strategy allows the design of macrolide derivatives that overcome antibiotic resistance. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, e2113632118.	3.3	7
2570	Investigating the interaction between organic anion transporter 1 and ochratoxin A: An in silico structural study to depict early molecular events of substrate recruitment and the impact of single point mutations. <i>Toxicology Letters</i> , 2022, 355, 19-30.	0.4	7
2571	Rhenium nanoparticles for the delivery of HSP 90 inhibitors: A new drug delivery platform designed by molecular dynamics simulation. <i>Journal of Molecular Liquids</i> , 2022, 347, 117995.	2.3	4
2573	Alpha-synuclein ϵ^{TM} in PreNAC(46-56) Fibril B ϵ^{TM} Molek ϵ^{TM} ler Dinamik Sim ϵ^{TM} lasyon Y ϵ^{TM} ntemi ile Konformasyonel De ϵ^{TM} erlendirmesi. <i>Kahramanmaraϵ^{TM} SAϵ^{TM} Aϵ^{TM} mam Aϵ^{TM}eniversitesi Tarϵ^{TM}m Ve Doϵ^{TM}ya Dergisi</i> , 0,2, .	0.2	1
2574	A structure model explaining the binding between a ubiquitous unconventional G-protein (OsYchF1) and a plant-specific C2-domain protein (OsGAP1) from rice. <i>Biochemical Journal</i> , 2020, 477, 3935-3949.	1.7	5
2576	Computing Potential of the Mean Force Profiles for Ion Permeation Through Channelrhodopsin Chimera, C1C2. <i>Methods in Molecular Biology</i> , 2021, 2191, 17-28.	0.4	3
2583	Computer Modeling of N-Acetylglutamate Synthase: From Primary Structure to Elemental Stages of Catalysis. <i>Doklady Biochemistry and Biophysics</i> , 2020, 495, 334-337.	0.3	1
2584	In silico prediction of ARB resistance: A first step in creating personalized ARB therapy. <i>PLoS Computational Biology</i> , 2020, 16, e1007719.	1.5	5
2586	Structural study of the G57W mutant of human gamma-S-crystallin, associated with congenital cataract. <i>Molecular Vision</i> , 2016, 22, 771-82.	1.1	5
2587	Modeling of the Binding of Peptide Blockers to Voltage-Gated Potassium Channels: Approaches and Evidence. <i>Acta Naturae</i> , 2016, 8, 35-46.	1.7	5
2588	Effect of monovalent salt concentration and peptide secondary structure in peptide-micelle binding. <i>RSC Advances</i> , 2021, 11, 36836-36849.	1.7	11
2589	A V(ϵ^{TM})-induced metallogel with solvent stimuli-responsive properties: structural proof-of-concept with MD simulations. <i>RSC Advances</i> , 2021, 11, 36801-36813.	1.7	1
2590	The structure of the <i>Aquifex aeolicus</i> MATE family multidrug resistance transporter and sequence comparisons suggest the existence of a new subfamily. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	5
2591	A Rationally and Computationally Designed Fluorescent Biosensor for ϵ^{TM} -Serine. <i>ACS Sensors</i> , 2021, 6, 4193-4205.	4.0	8

#	ARTICLE	IF	CITATIONS
2592	Mechanistic Picture for Monomeric Human Fibroblast Growth Factor 1 Stabilization by Heparin Binding. <i>Journal of Physical Chemistry B</i> , 2021, 125, 12690-12697.	1.2	4
2594	AMPA GluA2 subunit competitive inhibitors for PICK1 PDZ domain: Pharmacophore-based virtual screening, molecular docking, molecular dynamics simulation, and ADME studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 336-351.	2.0	1
2595	Analysis of L-DOPA and droxidopa binding to human β 2-adrenergic receptor. <i>Biophysical Journal</i> , 2021, , .	0.2	1
2596	Molecular dynamics study of hydrogen bond in peptide membrane at 150-300ÅK. <i>Journal of Molecular Liquids</i> , 2022, 349, 118165.	2.3	4
2597	Tracking the ATP-binding response in adenylate kinase in real time. <i>Science Advances</i> , 2021, 7, eabi5514.	4.7	18
2599	Molecular Simulations of Intrinsically Disordered Proteins and Their Binding Mechanisms. <i>Methods in Molecular Biology</i> , 2022, 2376, 343-362.	0.4	3
2600	Importance of Solvent in Guiding the Conformational Properties of an Intrinsically Disordered Peptide. <i>Langmuir</i> , 2021, 37, 14429-14442.	1.6	5
2601	A systematic drug repurposing approach to identify promising inhibitors from FDA-approved drugs against Nsp4 protein of SARS-CoV-2. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 550-559.	2.0	5
2602	Targeted Covalent Inhibitors Allosterically Deactivate the DEDDh Lassa Fever Virus NP Exonuclease from Alternative Distal Sites. <i>Jacs Au</i> , 2021, 1, 2315-2327.	3.6	3
2603	LSSmScarlet, dCyRFP2s, dCyOFP2s and CRISPRed2s, Genetically Encoded Red Fluorescent Proteins with a Large Stokes Shift. <i>International Journal of Molecular Sciences</i> , 2021, 22, 12887.	1.8	9
2604	ComplexMixtures.jl: Investigating the structure of solutions of complex-shaped molecules from a solvent-shell perspective. <i>Journal of Molecular Liquids</i> , 2022, 347, 117945.	2.3	16
2605	Vaccination in a humanized mouse model elicits highly protective PfCSP-targeting anti-malarial antibodies. <i>Immunity</i> , 2021, 54, 2859-2876.e7.	6.6	19
2606	A3 adenosine receptor agonists containing dopamine moieties for enhanced interspecies affinity. <i>European Journal of Medicinal Chemistry</i> , 2022, 228, 113983.	2.6	4
2608	Control of neurotransmitter release by two distinct membrane-binding faces of the Munc13-1 C1C2B region. <i>ELife</i> , 2021, 10, .	2.8	23
2609	The EGF Domains of MUC4 Oncomucin Mediate HER2 Binding Affinity and Promote Pancreatic Cancer Cell Tumorigenesis. <i>Cancers</i> , 2021, 13, 5746.	1.7	4
2610	Identification of Marine Fungi-Based Antiviral Agents as Potential Inhibitors of SARS-CoV-2 by Molecular Docking, ADMET and Molecular Dynamic Study. <i>Journal of Computational Biophysics and Chemistry</i> , 2022, 21, 139-153.	1.0	4
2611	Carbon Monoxide Binding to the Iron-Molybdenum Cofactor of Nitrogenase: a Detailed Quantum Mechanics/Molecular Mechanics Investigation. <i>Inorganic Chemistry</i> , 2021, 60, 18031-18047.	1.9	15
2612	Pressure Adaptations in Deep-Sea <i>Moritella</i> Dihydrofolate Reductases: Compressibility versus Stability. <i>Biology</i> , 2021, 10, 1211.	1.3	5

#	ARTICLE	IF	CITATIONS
2613	Simulation of pH-Dependent Conformational Transitions in Membrane Proteins: The CLC-ec1 Cl ⁻ /H ⁺ Antiporter. <i>Molecules</i> , 2021, 26, 6956.	1.7	4
2616	Functional Dynamics of an Ancient Membrane-Bound Hydrogenase. <i>Journal of the American Chemical Society</i> , 2021, , .	6.6	10
2617	Kinetic and structural mechanism for DNA unwinding by a non-hexameric helicase. <i>Nature Communications</i> , 2021, 12, 7015.	5.8	10
2618	Assessing the Intestinal Permeability of Small Molecule Drugs via Diffusion Motion on a Multidimensional Free Energy Surface. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 503-515.	2.3	10
2619	Cryo-EM reveals mechanistic insights into lipid-facilitated polyamine export by human ATP13A2. <i>Molecular Cell</i> , 2021, 81, 4799-4809.e5.	4.5	22
2620	Recharging your fats: CHARMM36 parameters for neutral lipids triacylglycerol and diacylglycerol. <i>Biophysical Reports</i> , 2021, 1, 100034.	0.7	10
2621	ChAdOx1 interacts with CAR and PF4 with implications for thrombosis with thrombocytopenia syndrome. <i>Science Advances</i> , 2021, 7, eabl8213.	4.7	112
2623	Temperature-Transferable Coarse-Grained Model for Poly(propylene oxide) to Study Thermo-Responsive Behavior of Triblock Copolymers. <i>Journal of Physical Chemistry B</i> , 2022, 126, 292-307.	1.2	6
2624	Small Amphiphilic Peptides: Activity Against a Broad Range of Drug-Resistant Bacteria and Structural Insight into Membranolytic Properties. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 665-687.	2.9	8
2625	Crystal structure and functional analysis of mycobacterial erythromycin resistance methyltransferase Erm38 reveals its RNA-binding site. <i>Journal of Biological Chemistry</i> , 2022, 298, 101571.	1.6	2
2626	Molecular dynamics study of the effects of static and oscillating electric fields in ovalbumin. <i>Innovative Food Science and Emerging Technologies</i> , 2022, 75, 102911.	2.7	12
2628	Mechanistic details of the actinobacterial lyase-catalyzed degradation reaction of 2-hydroxyisobutyryl-CoA. <i>Journal of Biological Chemistry</i> , 2022, 298, 101522.	1.6	2
2629	Synthesis & characterization of heterocyclic disazo - azomethine dyes and investigating their molecular docking & dynamics properties on acetylcholine esterase (AChE), heat shock protein (HSP90 α), nicotinamide N-methyl transferase (NNMT) and SARS-CoV-2 (2019-nCoV, COVID-19) main protease (Mpro). <i>Journal of Molecular Structure</i> , 2022, 1252, 131974.	1.8	7
2630	Computational Characterization of the Substrate Activation in the Active Site of SARS-CoV-2 Main Protease. <i>Supercomputing Frontiers and Innovations</i> , 2020, 7, .	0.5	1
2631	Atomistic Insights on the Adsorption of Long-Chain Undecane Molecules on Hydroxyl-Functionalized Carbon Nanotubes. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
2632	On the Adsorption of Volatile Organic Compounds on Hydroxyl-Functionalized Carbon Nanotubes in Aqueous Solution. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
2634	The Role of Triazole and Glucose Moieties in Alkali Metal Cation Complexation by Lower-Rim Tertiary-Amide Calix[4]arene Derivatives. <i>Molecules</i> , 2022, 27, 470.	1.7	4
2636	An Overview of Molecular Dynamics Simulation for Food Products and Processes. <i>Processes</i> , 2022, 10, 119.	1.3	16

#	ARTICLE	IF	CITATIONS
2637	Sequence coevolution and structure stabilization modulate olfactory receptor expression. <i>Biophysical Journal</i> , 2022, 121, 830-840.	0.2	4
2638	Do molecular dynamics force fields accurately model Ramachandran distributions of amino acid residues in water?. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3259-3279.	1.3	9
2639	A cost-effective water-in-salt electrolyte enables highly stable operation of a 2.15-V aqueous lithium-ion battery. <i>Cell Reports Physical Science</i> , 2022, 3, 100688.	2.8	16
2640	Hierarchical Self-Assembly Pathways of Peptoid Helices and Sheets. <i>Biomacromolecules</i> , 2022, 23, 992-1008.	2.6	19
2641	Immuno-Affinity Study of Oxidative Tyrosine Containing Peptides. <i>International Journal of Peptide Research and Therapeutics</i> , 2022, 28, 1.	0.9	1
2642	Aquaglyceroporin AQP7's affinity for its substrate glycerol. Have we reached convergence in the computed values of glycerol-aquaglyceroporin affinity?. <i>RSC Advances</i> , 2022, 12, 3128-3135.	1.7	4
2643	Structural insights on the effects of mutation of a charged binding pocket residue on phosphopeptide binding to 14-3-3 σ protein. <i>Proteins: Structure, Function and Bioinformatics</i> , 2022, 90, 1179-1189.	1.5	1
2645	Structural and functional insight into regulation of kinesin-1 by microtubule-associated protein MAP7. <i>Science</i> , 2022, 375, 326-331.	6.0	53
2646	Replica permutation with solute tempering for molecular dynamics simulation and its application to the dimerization of amyloid- β fragments. <i>Journal of Chemical Physics</i> , 2022, 156, 084109.	1.2	9
2647	Testing and Optimizing the Drude Polarizable Force Field for Blocked Amino Acids Based on High-Level Quantum-Mechanical Energy Surfaces. <i>Journal of Computational Biophysics and Chemistry</i> , 0, , 1-9.	1.0	3
2648	Helical structure motifs made searchable for functional peptide design. <i>Nature Communications</i> , 2022, 13, 102.	5.8	10
2649	Prediction of molecular interactions and physicochemical properties relevant for vasopressin V2 receptor antagonism. <i>Journal of Molecular Modeling</i> , 2022, 28, 31.	0.8	2
2650	Molecular descriptors suggest stapling as a strategy for optimizing membrane permeability of cyclic peptides. <i>Journal of Chemical Physics</i> , 2022, 156, 065101.	1.2	0
2651	Structure-mechanics statistical learning uncovers mechanical relay in proteins. <i>Chemical Science</i> , 2022, 13, 3688-3696.	3.7	4
2652	Computer Simulations of Deep Eutectic Solvents: Challenges, Solutions, and Perspectives. <i>International Journal of Molecular Sciences</i> , 2022, 23, 645.	1.8	46
2653	Structural Elements Directing G Proteins and β -Arrestin Interactions with the Human Melatonin Type 2 Receptor Revealed by Natural Variants. <i>ACS Pharmacology and Translational Science</i> , 2022, 5, 89-101.	2.5	2
2654	Molecular Determinants of Carbocation Cyclisation in Bacterial Monoterpene Synthases. <i>ChemBioChem</i> , 2022, 23, .	1.3	5
2656	Synthesis, Crystallographic, Quantum Chemical, Antitumor, and Molecular Docking/Dynamic Studies of 4-Hydroxycoumarin-Neurotransmitter Derivatives. <i>International Journal of Molecular Sciences</i> , 2022, 23, 1001.	1.8	31

#	ARTICLE	IF	CITATIONS
2657	Cytotoxic mechanism of tioconazole involves cell cycle arrest at mitosis through inhibition of microtubule assembly. <i>Cytotechnology</i> , 2022, 74, 141-162.	0.7	4
2658	Energetics and λ -coupling constants for Ala, Gly, and Val peptides demonstrated using ABEEM polarizable force field λ in vacuo and an aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 4232-4250.	1.3	1
2660	Identification of Structural transitions in bacterial fatty acid binding proteins that permit ligand entry and exit at membranes. <i>Journal of Biological Chemistry</i> , 2022, , 101676.	1.6	7
2661	Aggregation Behavior of Structurally Similar Therapeutic Peptides Investigated by ^1H NMR and All-Atom Molecular Dynamics Simulations. <i>Molecular Pharmaceutics</i> , 2022, 19, 904-917.	2.3	12
2663	Quantum Vibrational Spectroscopy of Explicitly Solvated Thymidine in Semiclassical Approximation. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 1350-1355.	2.1	8
2664	Molecular simulations of proteins: From simplified physical interactions to complex biological phenomena. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2022, 1870, 140757.	1.1	11
2665	Dynamics of electric field-controlled methotrexate delivery through membrane nanochannels. <i>Journal of Molecular Liquids</i> , 2022, 350, 118525.	2.3	0
2666	Predicting the evolution of number of native contacts of a small protein by using deep learning approach. <i>Computational Biology and Chemistry</i> , 2022, 97, 107625.	1.1	1
2667	Optimizing Lennard-Jones parameters by coupling single molecule and ensemble target data. <i>Computer Physics Communications</i> , 2022, 274, 108285.	3.0	1
2668	Envelope E protein of dengue virus and phospholipid binding to the late endosomal membrane. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2022, 1864, 183889.	1.4	9
2669	Accelerating the discovery of the beyond rule of five compounds that have high affinities toward SARS-CoV-2 spike RBD. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 2518-2527.	2.0	1
2670	Simultaneous parametrization of torsional and third-neighbor interaction terms in force-field development: The LLS-SC algorithm. <i>Journal of Computational Chemistry</i> , 2022, , .	1.5	1
2671	Ion permeation, selectivity, and electronic polarization in fluoride channels. <i>Biophysical Journal</i> , 2022, 121, 1336-1347.	0.2	12
2672	Pharmacophore modeling, Virtual screening, Molecular docking and dynamics studies for the discovery of HER2-tyrosine kinase inhibitors: An in-silico approach. <i>Journal of Molecular Structure</i> , 2022, , 132531.	1.8	8
2673	Drug Repurposing of the Unithiol: Inhibition of Metallo- β -Lactamases for the Treatment of Carbapenem-Resistant Gram-Negative Bacterial Infections. <i>International Journal of Molecular Sciences</i> , 2022, 23, 1834.	1.8	5
2674	Protein nanowires with tunable functionality and programmable self-assembly using sequence-controlled synthesis. <i>Nature Communications</i> , 2022, 13, 829.	5.8	30
2675	Bivalent recognition of fatty acyl-CoA by a human integral membrane palmitoyltransferase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	15
2676	Bridged Piperidine Analogues of a High Affinity Naphthalene-Based P2Y ₁₄ R Antagonist. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 3434-3459.	2.9	6

#	ARTICLE	IF	CITATIONS
2677	A Lead-Based Fragment Library Screening of the Glycosyltransferase WaaG from Escherichia coli. Pharmaceuticals, 2022, 15, 209.	1.7	3
2678	Identification of Halogen-Based Derivatives as Potent Inhibitors of Estrogen Receptor Alpha of Breast Cancer: An <i>In-Silico</i> Investigation. Journal of Computational Biophysics and Chemistry, 2022, 21, 181-205.	1.0	6
2679	Conformational transitions and ligand-binding to a muscle-type nicotinic acetylcholine receptor. Neuron, 2022, 110, 1358-1370.e5.	3.8	39
2680	Lateral access mechanism of LPA receptor probed by molecular dynamics simulation. PLoS ONE, 2022, 17, e0263296.	1.1	3
2681	Dynamics of the Histone Acetyltransferase Lysine-Rich Loop in the Catalytic Core of the CREB-Binding Protein. Journal of Chemical Information and Modeling, 2022, , .	2.5	3
2682	The complexin C-terminal amphipathic helix stabilizes the fusion pore open state by sculpting membranes. Nature Structural and Molecular Biology, 2022, 29, 97-107.	3.6	15
2683	Influence of Aqueous Arginine Solution on Regulating Conformational Stability and Hydration Properties of the Secondary Structural Segments of a Protein at Elevated Temperatures: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2022, 126, 1462-1476.	1.2	3
2684	Novel and Potential Small Molecule Scaffolds as DYRK1A Inhibitors by Integrated Molecular Docking-Based Virtual Screening and Dynamics Simulation Study. Molecules, 2022, 27, 1159.	1.7	8
2685	Insights on the proton translocation pathways in F ₁ F ₀ -ATP synthase using molecular dynamics simulations. Archives of Biochemistry and Biophysics, 2022, 717, 109135.	1.4	3
2686	A unifying framework for amyloid-mediated membrane damage: The lipid-chaperone hypothesis. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2022, 1870, 140767.	1.1	15
2687	Martini 3 Coarse-Grained Model for Type III Deep Eutectic Solvents: Thermodynamic, Structural, and Extraction Properties. ACS Sustainable Chemistry and Engineering, 2021, 9, 17338-17350.	3.2	20
2688	Structural basis of sphingosine-1-phosphate receptor 1 activation and biased agonism. Nature Chemical Biology, 2022, 18, 281-288.	3.9	43
2689	Effect of dopamine-functionalization, charge and pH on protein corona formation around TiO ₂ nanoparticles. Nanoscale, 2022, 14, 5121-5137.	2.8	10
2690	Exploring the trimerization process of a transmembrane helix with an ionizable residue by molecular dynamics simulations: a case study of transmembrane domain 5 of LMP-1. Physical Chemistry Chemical Physics, 2022, 24, 7084-7092.	1.3	0
2691	Extended-ensemble docking to probe dynamic variation of ligand binding sites during large-scale structural changes of proteins. Chemical Science, 2022, 13, 4150-4169.	3.7	7
2692	Characterization of Amyloidogenic Peptide Aggregability in Helical Subspace. Methods in Molecular Biology, 2022, 2340, 401-448.	0.4	3
2693	Evidence for a trap-and-flip mechanism in a proton-dependent lipid transporter. Nature Communications, 2022, 13, 1022.	5.8	10
2694	Identification of new putative inhibitors of <i>Mycobacterium tuberculosis</i> 3-dehydroshikimate dehydratase from a combination of ligand- and structure-based and deep learning <i>in silico</i> approaches. Journal of Biomolecular Structure and Dynamics, 2023, 41, 2971-2980.	2.0	5

#	ARTICLE	IF	CITATIONS
2695	Isolation and In Silico Anti-SARS-CoV-2 Papain-Like Protease Potentialities of Two Rare 2-Phenoxychromone Derivatives from <i>Artemisia</i> spp.. <i>Molecules</i> , 2022, 27, 1216.	1.7	27
2696	Evolutionary information helps understand distinctive features of the angiotensin II receptors AT1 and AT2 in amniota. <i>PLoS Computational Biology</i> , 2022, 18, e1009732.	1.5	0
2697	Microscopic Characterization of the Chloride Permeation Pathway in the Human Excitatory Amino Acid Transporter 1 (EAAT1). <i>ACS Chemical Neuroscience</i> , 2022, 13, 776-785.	1.7	6
2698	Factors That Determine the Variation of Equilibrium and Kinetic Properties of QM/MM Enzyme Simulations: QM Region, Conformation, and Boundary Condition. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2530-2542.	2.3	9
2699	Allosteric Determinants of the SARS-CoV-2 Spike Protein Binding with Nanobodies: Examining Mechanisms of Mutational Escape and Sensitivity of the Omicron Variant. <i>International Journal of Molecular Sciences</i> , 2022, 23, 2172.	1.8	5
2700	Specificity of <i>Loxosceles</i> ð± clade phospholipase D enzymes for choline-containing lipids: Role of a conserved aromatic cage. <i>PLoS Computational Biology</i> , 2022, 18, e1009871.	1.5	6
2701	Coexistence of Ammonium Transporter and Channel Mechanisms in Amt-Mep-Rh Twin-His Variants Impairs the Filamentation Signaling Capacity of Fungal Mep2 Transceptors. <i>MBio</i> , 2022, 13, e0291321.	1.8	6
2702	Binding and Activation of Serotonergic G-Protein Coupled Receptors by the Multimodal Antidepressant Vortioxetine. <i>ACS Chemical Neuroscience</i> , 2022, 13, 1129-1142.	1.7	1
2703	Water Distribution on Protein Surface of the Lyophilized Proteins With Different Topography Studied by Molecular Dynamics Simulations. <i>Journal of Pharmaceutical Sciences</i> , 2022, 111, 2299-2311.	1.6	0
2704	Ligand and Structure-Based In Silico Determination of the Most Promising SARS-CoV-2 nsp16-nsp10 2â€²-o-Methyltransferase Complex Inhibitors among 3009 FDA Approved Drugs. <i>Molecules</i> , 2022, 27, 2287.	1.7	34
2706	Construction and Application of a High-Throughput <i>In Vivo</i> Screening Platform for the Evolution of Nitrile Metabolism-Related Enzymes Based on a Desensitized Repressive Biosensor. <i>ACS Synthetic Biology</i> , 2022, 11, 1577-1587.	1.9	7
2707	Interconversion between Serum Amyloid A Native and Fibril Conformations. <i>ACS Omega</i> , 2022, 7, 12186-12192.	1.6	2
2708	In silico evidence for prednisone and progesterone efficacy in recurrent implantation failure treatment. <i>Journal of Molecular Modeling</i> , 2022, 28, 105.	0.8	3
2709	Molecular Dynamics-Assisted Optimization of Protein NMR Relaxation Analysis. <i>Journal of Chemical Theory and Computation</i> , 2022, , .	2.3	2
2710	Integration of experimental data and use of automated fitting methods in developing protein force fields. <i>Communications Chemistry</i> , 2022, 5, .	2.0	12
2712	Unraveling Flow Separation at the Waterâ€™Carbon Nanotube Interface: An Atomic-Scale Overview by Molecular Dynamics Simulation. <i>Langmuir</i> , 2022, , .	1.6	2
2714	Dimerization of the Peptide CXCR4-Antagonist on Macromolecular and Supramolecular Protraction Arms Affords Increased Potency and Enhanced Plasma Stability. <i>Bioconjugate Chemistry</i> , 2022, 33, 594-607.	1.8	5
2715	Ligand-Dependent Modulation of the Dynamics of Intracellular Loops Dictates Functional Selectivity of 5-HT _{2A} R. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2522-2537.	2.5	5

#	ARTICLE	IF	CITATIONS
2716	Modeling the membrane binding mechanism of a lipid transport protein Osh4 to single membranes. <i>Biophysical Journal</i> , 2022, 121, 1560-1575.	0.2	4
2717	Stiffening Effect of Ceramide on Lipid Membranes Provides Non-Sacrificial Protection against Potent Chemical Damage. <i>Langmuir</i> , 2022, 38, 3522-3529.	1.6	1
2718	Large Area Covalent Organic Polymers Membrane via Sol-Gel Approach for Harvesting the Salinity Gradient Energy. <i>Small</i> , 2022, 18, e2107600.	5.2	13
2719	Isolation and In Silico SARS-CoV-2 Main Protease Inhibition Potential of Jusan Coumarin, a New Dicomarin from <i>Artemisia glauca</i> . <i>Molecules</i> , 2022, 27, 2281.	1.7	16
2720	A distinct mechanism of C-type inactivation in the Kv-like KcsA mutant E71V. <i>Nature Communications</i> , 2022, 13, 1574.	5.8	11
2721	Devising Bone Molecular Models at the Nanoscale: From Usual Mineralized Collagen Fibrils to the First Bone Fibers Including Hydroxyapatite in the Extra-Fibrillar Volume. <i>Materials</i> , 2022, 15, 2274.	1.3	4
2722	Jusanin, a New Flavonoid from <i>Artemisia commutata</i> with an In Silico Inhibitory Potential against the SARS-CoV-2 Main Protease. <i>Molecules</i> , 2022, 27, 1636.	1.7	23
2723	Complex of HIV-1 Integrase with Cellular Ku Protein: Interaction Interface and Search for Inhibitors. <i>International Journal of Molecular Sciences</i> , 2022, 23, 2908.	1.8	4
2724	A molecular switch controls the impact of cholesterol on a Kir channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2109431119.	3.3	9
2725	Virtual screening, optimization and molecular dynamics analyses highlighting a pyrrolo[1,2-a]quinazoline derivative as a potential inhibitor of DNA gyrase B of <i>Mycobacterium tuberculosis</i> . <i>Scientific Reports</i> , 2022, 12, 4742.	1.6	15
2727	Modelling Protein Plasticity: The Example of Frataxin and Its Variants. <i>Molecules</i> , 2022, 27, 1955.	1.7	2
2728	Optimizing Multisite π -Dynamics Throughput with Charge Renormalization. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1479-1488.	2.5	8
2729	Multi-Phase In Silico Discovery of Potential SARS-CoV-2 RNA-Dependent RNA Polymerase Inhibitors among 3009 Clinical and FDA-Approved Related Drugs. <i>Processes</i> , 2022, 10, 530.	1.3	29
2730	The Mechanism of Action of Hepatitis B Virus Capsid Assembly Modulators Can Be Predicted from Binding to Early Assembly Intermediates. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 4854-4864.	2.9	8
2731	Alchemical Free Energy Methods Applied to Complexes of the First Bromodomain of BRD4. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1458-1470.	2.5	8
2732	A Computational Understanding of Inter-Individual Variability in CYP2D6 Activity to Investigate the Impact of Missense Mutations on Ochratoxin A Metabolism. <i>Toxins</i> , 2022, 14, 207.	1.5	5
2733	Dynamic Heterogeneity at the Interface of an Intrinsically Disordered Peptide. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1942-1955.	2.5	6
2734	MutCov: A pipeline for evaluating the effect of mutations in spike protein on infectivity and antigenicity of SARS-CoV-2. <i>Computers in Biology and Medicine</i> , 2022, 145, 105509.	3.9	2

#	ARTICLE	IF	CITATIONS
2735	The lung surfactant activity probed with molecular dynamics simulations. <i>Advances in Colloid and Interface Science</i> , 2022, 304, 102659.	7.0	6
2736	Ataxia-linked SLC1A3 mutations alter EAAT1 chloride channel activity and glial regulation of CNS function. <i>Journal of Clinical Investigation</i> , 2022, 132, .	3.9	10
2737	The Transition of Photoreceptor Guanylate Cyclase Type 1 to the Active State. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4030.	1.8	1
2738	On the adsorption of volatile organic compounds on hydroxyl-functionalized carbon nanotubes in aqueous solution. <i>Diamond and Related Materials</i> , 2022, 125, 108994.	1.8	7
2739	Understanding ion-ion and ion-solvent interactions in aqueous solutions of morpholinium ionic liquids with N-acetyl-L-alanine anion through partial molar properties and molecular dynamics simulations. <i>Journal of Molecular Liquids</i> , 2022, 354, 118876.	2.3	2
2740	Allosteric modulation of the chemokine receptor-chemokine CXCR4-CXCL12 complex by tyrosine sulfation. <i>International Journal of Biological Macromolecules</i> , 2022, 206, 812-822.	3.6	4
2741	Crystal structures of TTHA1265 and TTHA1264/TTHA1265 complex reveal an intrinsic heterodimeric assembly. <i>International Journal of Biological Macromolecules</i> , 2022, 207, 424-433.	3.6	0
2742	Water structure in glycerol: Spectroscopic and computer simulation investigation of hydrogen bonding and water clustering. <i>Journal of Molecular Liquids</i> , 2022, 355, 118916.	2.3	8
2743	WIND-PVPA: Water/Ion NMR Detected PVPA to assess lipid barrier integrity in vitro through quantification of passive water- and ion transport. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2022, 1864, 183911.	1.4	3
2744	In vitro, in vivo and in silico evaluation of the anti-inflammatory potential of <i>Hyssopus officinalis</i> L. subsp. <i>aristatus</i> (Godr.) Nyman (Lamiaceae). <i>Journal of Ethnopharmacology</i> , 2022, 293, 115201.	2.0	10
2745	Molecular Simulation of Stapled Peptides. <i>Methods in Molecular Biology</i> , 2022, 2405, 283-301.	0.4	1
2746	CHARMM-GUI Nanomaterial Modeler for Modeling and Simulation of Nanomaterial Systems. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 479-493.	2.3	53
2747	The role of cysteine residues in the allosteric modulation of the chromophore phototransformations of biphotochromic fluorescent protein SAASoti. <i>Scientific Reports</i> , 2021, 11, 24314.	1.6	5
2750	Mutants only partially represent characteristics of calcium-release-activated calcium channel gating. <i>Chinese Journal of Chemical Physics</i> , 2021, 34, 915-924.	0.6	0
2752	Modelling of the Citrus CCD4 Family Members: In Silico Analysis of Membrane Binding and Substrate Preference. <i>International Journal of Molecular Sciences</i> , 2021, 22, 13616.	1.8	2
2753	Enhanced Conformational Sampling of Nanobody CDR H3 Loop by Generalized Replica-Exchange with Solute Tempering. <i>Life</i> , 2021, 11, 1428.	1.1	2
2757	<sc>CHARMM-GUI</sc> Drude preppep for molecular dynamics simulation using the classical Drude polarizable force field. <i>Journal of Computational Chemistry</i> , 2022, 43, 359-375.	1.5	24
2758	Asymmetric drug binding in an ATP-loaded inward-facing state of an ABC transporter. <i>Nature Chemical Biology</i> , 2022, 18, 226-235.	3.9	15

#	ARTICLE	IF	CITATIONS
2759	Plasticity within the barrel domain of BamA mediates a hybrid-barrel mechanism by BAM. <i>Nature Communications</i> , 2021, 12, 7131.	5.8	34
2760	On-the-fly adiabatically switched semiclassical initial value representation molecular dynamics for vibrational spectroscopy of biomolecules. <i>Journal of Chemical Physics</i> , 2021, 155, 234102.	1.2	13
2761	How Much Entropy Is Contained in NMR Relaxation Parameters?. <i>Journal of Physical Chemistry B</i> , 2022, 126, 54-68.	1.2	17
2762	Retinal Vibrations in Bacteriorhodopsin are Mechanically Harmonic but Electrically Anharmonic: Evidence From Overtone and Combination Bands. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 749261.	1.6	3
2764	Towards Computationally Guided Design and Engineering of a <i>Neisseria meningitidis</i> Serogroup W Capsule Polymerase with Altered Substrate Specificity. <i>Processes</i> , 2021, 9, 2192.	1.3	2
2765	Structure and ion-release mechanism of PIB-4-type ATPases. <i>ELife</i> , 2021, 10, .	2.8	8
2766	Pyranose Ring Puckering Thermodynamics for Glycan Monosaccharides Associated with Vertebrate Proteins. <i>International Journal of Molecular Sciences</i> , 2022, 23, 473.	1.8	11
2767	Drug Repurposing for Influenza Virus Polymerase Acidic (PA) Endonuclease Inhibitor. <i>Molecules</i> , 2021, 26, 7326.	1.7	3
2768	Altering the Double-Stranded DNA Specificity of the bZIP Domain of Zta with Site-Directed Mutagenesis at N182. <i>ACS Omega</i> , 2022, 7, 129-139.	1.6	0
2769	Precise druggability of the PTH type 1 receptor. <i>Nature Chemical Biology</i> , 2022, 18, 272-280.	3.9	11
2770	Distinguishing between Similar Miniproteins with Single-Molecule Nanopore Sensing: A Computational Study. <i>ACS Nanoscience Au</i> , 2022, 2, 119-127.	2.0	1
2772	Computer Simulations and Network-Based Profiling of Binding and Allosteric Interactions of SARS-CoV-2 Spike Variant Complexes and the Host Receptor: Dissecting the Mechanistic Effects of the Delta and Omicron Mutations. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4376.	1.8	16
2773	Production of \hat{I}^2 -keto adipic acid from glucose in <i>Pseudomonas putida</i> KT2440 for use in performance-advantaged nylons. <i>Cell Reports Physical Science</i> , 2022, 3, 100840.	2.8	18
2775	Computational design of stapled peptide inhibitor against SARS-CoV-2 receptor binding domain. <i>Peptide Science</i> , 2022, 114, e24267.	1.0	8
2776	SPICA Force Field for Proteins and Peptides. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3204-3217.	2.3	21
2777	Structural Characterization of the Full-Length Anti-CD20 Antibody Rituximab. <i>Frontiers in Molecular Biosciences</i> , 2022, 9, 823174.	1.6	10
2779	Global Fold Switching of the RafH Protein: Diverse Structures with a Conserved Pathway. <i>Journal of Physical Chemistry B</i> , 2022, 126, 2979-2989.	1.2	2
2780	Review on the QM/MM Methodologies and Their Application to Metalloproteins. <i>Molecules</i> , 2022, 27, 2660.	1.7	28

#	ARTICLE	IF	CITATIONS
2781	Nâ€²-terminal- and Ca ²⁺ -induced stabilization of high-order oligomers of full-length Danio rerio and Homo sapiens otolin-1. <i>International Journal of Biological Macromolecules</i> , 2022, 209, 1032-1047.	3.6	2
2782	The SARS-CoV-2 helicase as a target for antiviral therapy: Identification of potential small molecule inhibitors by in silico modelling. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 114, 108193.	1.3	8
2783	Structural basis for the assembly and quinone transport mechanisms of the dimeric photosynthetic RCâ€“LH1 supercomplex. <i>Nature Communications</i> , 2022, 13, 1977.	5.8	22
2784	Changes in Salt Concentration Modify the Translocation of Neutral Molecules through a Î”CymA Nanopore in a Non-monotonic Manner. <i>ACS Nano</i> , 2022, 16, 7701-7712.	7.3	6
2785	Thermostabilizing ketoreductase ChKRED20 by consensus mutagenesis at dimeric interfaces. <i>Enzyme and Microbial Technology</i> , 2022, 158, 110052.	1.6	4
2786	Physicochemical Properties Altered by the Tail Group of Lipid Membranes Influence Huntingtin Aggregation and Lipid Binding. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3067-3081.	1.2	6
2839	Millisecond molecular dynamics simulations of KRas-dimer formation and interfaces. <i>Biophysical Journal</i> , 2022, 121, 3730-3744.	0.2	6
2840	Molecular Basis for the Cation Selectivity of Salmonella typhimurium Melibiose Permease. <i>Journal of Molecular Biology</i> , 2022, 434, 167598.	2.0	7
2841	NMR Provides Unique Insight into the Functional Dynamics and Interactions of Intrinsically Disordered Proteins. <i>Chemical Reviews</i> , 2022, 122, 9331-9356.	23.0	51
2842	Nanovectorization of Ivermectin to avoid overdose of drugs. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 4272-4285.	2.0	0
2843	Structure of the Shaker Kv channel and mechanism of slow C-type inactivation. <i>Science Advances</i> , 2022, 8, eabm7814.	4.7	49
2844	A threefold approach including quantum chemical, molecular docking and molecular dynamic studies to explore the natural compounds from Centaurea jacea as the potential inhibitors for COVID-19. <i>Brazilian Journal of Biology</i> , 2021, 83, e247604.	0.4	3
2845	Kinks in buckled graphene uncompressed and compressed in the longitudinal direction. <i>Theoretical and Computational Chemistry</i> , 2022, , 41-60.	0.2	0
2846	Identification of the probable structure of the sAPP ^{Î±} -GABA _B R1a complex and theoretical solutions for such cases. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12267-12280.	1.3	6
2847	Spontaneous Reactivation of OPC-Inhibited BChE Mutants: Modeling of Mechanisms. <i>Russian Journal of Physical Chemistry B</i> , 2022, 16, 103-108.	0.2	3
2848	A Puzzling Protein from <i>Variovorax paradoxus</i> Has a PLP Fold Type IV Transaminase Structure and Binds PLP without Catalytic Lysine. <i>Crystals</i> , 2022, 12, 619.	1.0	0
2849	Computation of the Protein Conformational Transition Pathway on Ligand Binding by Linear Response-Driven Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3268-3283.	2.3	5
2850	Ion behavior in the selectivity filter of HCN1 channels. <i>Biophysical Journal</i> , 2022, , .	0.2	3

#	ARTICLE	IF	CITATIONS
2851	Delineating the Mechanism of Action of a Protease Resistant and Salt Tolerant Synthetic Antimicrobial Peptide against <i>Pseudomonas aeruginosa</i> . ACS Omega, 2022, 7, 15951-15968.	1.6	6
2852	Rate-limiting transport of positively charged arginine residues through the Sec-machinery is integral to the mechanism of protein secretion. ELife, 2022, 11, .	2.8	13
2853	Peptidoglycan biosynthesis is driven by lipid transfer along enzyme-substrate affinity gradients. Nature Communications, 2022, 13, 2278.	5.8	20
2854	Information flow and allosteric communication in proteins. Journal of Chemical Physics, 2022, 156, 185101.	1.2	2
2855	Molecular Dynamics of DHHC20 Acyltransferase Suggests Principles of Lipid and Protein Substrate Selectivity. International Journal of Molecular Sciences, 2022, 23, 5091.	1.8	6
2856	Magic mushroom extracts in lipid membranes. Biochimica Et Biophysica Acta - Biomembranes, 2022, 1864, 183957.	1.4	5
2857	First biphotochromic fluorescent protein moxSAASoti stabilized for oxidizing environment. Scientific Reports, 2022, 12, 7862.	1.6	1
2858	How Does Temperature Affect the Dynamics of SARS-CoV-2 M Proteins? Insights from Molecular Dynamics Simulations. Journal of Membrane Biology, 2022, 255, 341-356.	1.0	3
2859	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. International Journal of Molecular Sciences, 2022, 23, 5449.	1.8	1
2860	Toward the Discovery of a Novel Class of Leads for High Altitude Disorders by Virtual Screening and Molecular Dynamics Approaches Targeting Carbonic Anhydrase. International Journal of Molecular Sciences, 2022, 23, 5054.	1.8	13
2861	Molecular dynamics simulation of interaction between nanorod and phospholipid molecules bilayer. Chinese Physics B, 2023, 32, 016201.	0.7	2
2862	SARS-CoV-2 Delta Variant Decreases Nanobody Binding and ACE2 Blocking Effectivity. Journal of Chemical Information and Modeling, 2022, , .	2.5	5
2863	Structural dynamics of SARS-CoV-2 nucleocapsid protein induced by RNA binding. PLoS Computational Biology, 2022, 18, e1010121.	1.5	19
2864	Mechanistic basis for multidrug resistance and collateral drug sensitivity conferred to the malaria parasite by polymorphisms in PfMDR1 and PfCRT. PLoS Biology, 2022, 20, e3001616.	2.6	15
2865	Development of novel monoamine oxidase B (MAO-B) inhibitors by combined application of docking-based alignment, 3D-QSAR, ADMET prediction, molecular dynamics simulation, and MM_GBSA binding free energy. Journal of Biomolecular Structure and Dynamics, 2023, 41, 4667-4680.	2.0	12
2866	Miniature β -Hairpin Mimetic by Intramolecular Hydrogen Bond and C-H \cdots N Interactions. ACS Omega, 0, , .	1.6	2
2867	A 300-fold conductivity increase in microbial cytochrome nanowires due to temperature-induced restructuring of hydrogen bonding networks. Science Advances, 2022, 8, eabm7193.	4.7	28
2868	Investigation of the structural and dynamical properties of human uncoupling protein 2 through molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2022, 114, 108203.	1.3	2

#	ARTICLE	IF	CITATIONS
2869	Statistical and energetic analysis of hydrogen bonds in short and long peptide nanotapes/nanofibers using molecular dynamics simulations. <i>Journal of Molecular Liquids</i> , 2022, 359, 119308.	2.3	4
2870	Cooperative antimicrobial action of melittin on lipid membranes: A coarse-grained molecular dynamics study. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2022, 1864, 183955.	1.4	10
2871	Benchmarking Adaptive Steered Molecular Dynamics (ASMD) on CHARMM Force Fields. <i>ChemPhysChem</i> , 2022, 23, .	1.0	3
2872	Free-Energy Surfaces of Two Cardiac Thin Filament Conformational Changes during Muscle Contraction. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3844-3851.	1.2	4
2873	Developing a Rational Approach to Designing Recombinant Proteins for Peptide-Directed Nanoparticle Synthesis. <i>Nanoscale Advances</i> , 0, , .	2.2	4
2875	Temporin B Forms Hetero-Oligomers with Temporin L, Modifies Its Membrane Activity, and Increases the Cooperativity of Its Antibacterial Pharmacodynamic Profile. <i>Biochemistry</i> , 2022, 61, 1029-1040.	1.2	5
2876	Osteogenic growth peptide is a potent anti-inflammatory and bone preserving hormone via cannabinoid receptor type 2. <i>ELife</i> , 0, 11, .	2.8	6
2877	Influence of the leaving group on the mechanism of hydrolysis of organophosphorus compounds by phosphotriesterase from bacterium <i>Pseudomonas diminuta</i> . <i>Russian Chemical Bulletin</i> , 2022, 71, 921-926.	0.4	1
2879	Elucidating the molecular basis of spontaneous activation in an engineered mechanosensitive channel. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 2539-2550.	1.9	5
2880	py-MCMD: Python Software for Performing Hybrid Monte Carlo/Molecular Dynamics Simulations with GOMC and NAMD. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4983-4994.	2.3	10
2881	Differential ion dehydration energetics explains selectivity in the non-canonical lysosomal K ⁺ channel TMEM175. <i>ELife</i> , 0, 11, .	2.8	9
2882	Nanomechanics combined with HDX reveals allosteric drug binding sites of CFTR NBD1. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 2587-2599.	1.9	1
2884	Insilico structure based drug design approach to find potential hits in ventilator-associated pneumonia caused by <i>Pseudomonas aeruginosa</i> . <i>Computers in Biology and Medicine</i> , 2022, 146, 105597.	3.9	0
2885	Tunnels Connect Lipid Bilayer to Occluded Odorant-Binding Sites of Insect Olfactory Receptor. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
2887	Computational functional analysis of cysteine residues in proteins. , 2022, , 59-80.		2
2888	Mechanistic Insights into Enzyme Catalysis from Explaining Machine-Learned Quantum Mechanical and Molecular Mechanical Minimum Energy Pathways. <i>ACS Physical Chemistry Au</i> , 2022, 2, 316-330.	1.9	5
2889	A topological refactoring design strategy yields highly stable granulopoietic proteins. <i>Nature Communications</i> , 2022, 13, .	5.8	4
2890	Influence of Ion Specificity and Concentration on the Conformational Transition of Intrinsically Disordered Sheep Prion Peptide. <i>ChemPhysChem</i> , 2022, 23, .	1.0	3

#	ARTICLE	IF	CITATIONS
2891	Edge weights in a protein elastic network reorganize collective motions and render long-range sensitivity responses. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	2
2894	Significant Improvement of Both Catalytic Efficiency and Stability of Fructosyltransferase from <i>Aspergillus niger</i> by Structure-Guided Engineering of Key Residues in the Conserved Sequence of the Catalytic Domain. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 7202-7210.	2.4	13
2896	Bacterial H-NS contacts DNA at the same irregularly spaced sites in both bridged and hemi-sequestered linear filaments. <i>IScience</i> , 2022, 25, 104429.	1.9	7
2898	Quantitative characterization of the path of glucose diffusion facilitated by human glucose transporter 1. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2022, 1864, 183975.	1.4	1
2899	HIV-1 mutants that escape the cytotoxic T-lymphocytes are defective in viral DNA integration. , 2022, 1, .		5
2902	Phosphorylation Induced Conformational Transitions in DNA Polymerase β . <i>Frontiers in Molecular Biosciences</i> , 0, 9, .	1.6	2
2903	Structural basis of human ACE2 higher binding affinity to currently circulating Omicron SARS-CoV-2 sub-variants BA.2 and BA.1.1. <i>Cell</i> , 2022, 185, 2952-2960.e10.	13.5	96
2904	Protein-Nucleic Acid Interactions for RNA Polymerase II Elongation Factors by Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3079-3089.	2.5	6
2908	Insighting isatin derivatives as potential antiviral agents against NSP3 of COVID-19. <i>Chemical Papers</i> , 2022, 76, 6271-6285.	1.0	6
2909	The Antifreeze and Cryoprotective Activities of a Novel Antifreeze Peptide from <i>Ctenopharyngodon idella</i> Scales. <i>Foods</i> , 2022, 11, 1830.	1.9	2
2910	Graph-learning guided mechanistic insights into imipenem hydrolysis in GES carbapenemases. <i>Electronic Structure</i> , 2022, 4, 034001.	1.0	2
2912	Computing transition path theory quantities with trajectory stratification. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	8
2913	Characterization of the membrane interactions of phospholipase $C\beta$ reveals key features of the active enzyme. <i>Science Advances</i> , 2022, 8, .	4.7	7
2916	<i>PcoB</i> is a defense outer membrane protein that facilitates cellular uptake of copper. <i>Protein Science</i> , 2022, 31, .	3.1	5
2917	Interfacial Water in the SARS Spike Protein: Investigating the Interaction with Human ACE2 Receptor and In Vitro Uptake in A549 Cells. <i>Langmuir</i> , 2022, 38, 7976-7988.	1.6	20
2919	Computational Reconstruction and Analysis of Structural Models of Avian Cryptochrome 4. <i>Journal of Physical Chemistry B</i> , 2022, 126, 4623-4635.	1.2	11
2921	Assessment of the Components of the Electrostatic Potential of Proteins in Solution: Comparing Experiment and Theory. <i>Journal of Physical Chemistry B</i> , 2022, 126, 4543-4554.	1.2	8
2922	Enhanced-Sampling Simulations for the Estimation of Ligand Binding Kinetics: Current Status and Perspective. <i>Frontiers in Molecular Biosciences</i> , 0, 9, .	1.6	24

#	ARTICLE	IF	CITATIONS
2923	Interplay between the Enamine and Imine Forms of the Hydrolyzed Imipenem in the Active Sites of Metallo- β -lactamases and in Water Solution. <i>Journal of Chemical Information and Modeling</i> , 0, , .	2.5	3
2924	Computational Study of the Allosteric Effects of p5 on CDK5's p25 Hyperactivity as Alternative Inhibitory Mechanisms in Neurodegeneration. <i>Journal of Physical Chemistry B</i> , 2022, 126, 5033-5044.	1.2	2
2925	Design, Synthesis, In Silico and In Vitro Studies of New Immunomodulatory Anticancer Nicotinamide Derivatives Targeting VEGFR-2. <i>Molecules</i> , 2022, 27, 4079.	1.7	10
2926	Atomistic insight into the luminal allosteric regulation of vesicular glutamate transporter 2 by chloride and protons: An <i>in-silico</i> molecular dynamics simulation study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2022, 90, 2045-2057.	1.5	2
2927	Homology modeling, virtual screening, molecular docking, molecular dynamic (MD) simulation, and ADMET approaches for identification of natural anti-Parkinson agents targeting MAO-B protein. <i>Neuroscience Letters</i> , 2022, 786, 136803.	1.0	6
2928	Exploring CRD mobility during RAS/RAF engagement at the membrane. <i>Biophysical Journal</i> , 2022, 121, 3630-3650.	0.2	9
2929	Conformational selection guides β -arrestin recruitment at a biased G protein-coupled receptor. <i>Science</i> , 2022, 377, 222-228.	6.0	16
2930	On the force field optimisation of β -lactam cores using the force field Toolkit. <i>Journal of Computer-Aided Molecular Design</i> , 0, , .	1.3	0
2931	Effect of Leu/Val Mutation on the Energetics of Antimicrobial Peptide: Micelle Binding. <i>Journal of Physical Chemistry B</i> , 2022, 126, 5262-5273.	1.2	2
2932	Procyanidin C1 Location, Interaction, and Aggregation in Two Complex Biomembranes. <i>Membranes</i> , 2022, 12, 692.	1.4	1
2934	The Role of Extracellular Loops in the Folding of Outer Membrane Protein X (OmpX) of <i>Escherichia coli</i> . <i>Frontiers in Molecular Biosciences</i> , 0, 9, .	1.6	3
2935	Implementation of Telescoping Boxes in Adaptive Steered Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4649-4659.	2.3	8
2936	Resolution exchange with tunneling for enhanced sampling of protein landscapes. <i>Physical Review E</i> , 2022, 106, .	0.8	1
2938	MD simulation-based screening approach identified tolvaptan as a potential inhibitor of Eg5. <i>Molecular Diversity</i> , 2023, 27, 1203-1221.	2.1	1
2939	Computational Assessment of Protein-Protein Binding Specificity within a Family of Synaptic Surface Receptors. <i>Journal of Physical Chemistry B</i> , 2022, 126, 7510-7527.	1.2	6
2940	Design and synthesis of thiazolidine-2,4-diones hybrids with 1,2-dihydroquinolones and 2-oxindoles as potential VEGFR-2 inhibitors: <i>in-vitro</i> anticancer evaluation and <i>in-silico</i> studies. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2022, 37, 1903-1917.	2.5	64
2941	Hyper-swivel head domain motions are required for complete mRNA-tRNA translocation and ribosome resetting. <i>Nucleic Acids Research</i> , 2022, 50, 8302-8320.	6.5	3
2943	A Multi-Scale Approach to Model K ⁺ Permeation Through the KcsA Channel. <i>Frontiers in Molecular Biosciences</i> , 0, 9, .	1.6	2

#	ARTICLE	IF	CITATIONS
2944	Modeling Gd ³⁺ Complexes for Molecular Dynamics Simulations: Toward a Rational Optimization of MRI Contrast Agents. <i>Inorganic Chemistry</i> , 2022, 61, 11837-11858.	1.9	3
2946	A rationale for the unlike potency of avibactam and ETX2514 against OXA-24 β -lactamase. <i>Archives of Biochemistry and Biophysics</i> , 2022, 727, 109343.	1.4	1
2947	Evaluation of interaction between Ponceau 4R (P4R) and trypsin using kinetic, spectroscopic, and molecular dynamics simulation methods. <i>Journal of Molecular Liquids</i> , 2022, 362, 119761.	2.3	3
2948	The roles of functional groups of antifreeze protein in inhibition of hydrate growth. <i>Fuel</i> , 2022, 327, 125060.	3.4	10
2949	An efficient pTSA catalyzed synthesis of some new substituted 5-hydroxy-3-phenylisoxazol-4-yl-1,3-dimethyl-1H-chromeno[2,3-d]pyrimidine-2,4(3H,5H)-dione/3,3-dimethyl-1H-chromeno[2,3-d]pyrimidine-2,4(3H,5H)-dione scaffolds and evaluation of their pharmacological and computational investigations. <i>Journal of Molecular Structure</i> , 2022, 1267, 133587.	1.8	7
2950	Molecular dynamics simulations of cRGD-conjugated PEGylated TiO ₂ nanoparticles for targeted photodynamic therapy. <i>Journal of Colloid and Interface Science</i> , 2022, 627, 126-141.	5.0	8
2951	Identification of Small-Molecule Inhibitors of Fibroblast Growth Factor 23 Signaling via In Silico Hot Spot Prediction and Molecular Docking to \pm -Klotho. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3627-3637.	2.5	5
2953	The same, but different, but still the same: structural and dynamical differences of neutrophil elastase and cathepsin G. <i>European Physical Journal D</i> , 2022, 76, .	0.6	1
2954	Charge-based interactions through peptide position 4 drive diversity of antigen presentation by human leukocyte antigen class I molecules. , 2022, 1, .		3
2955	Structural basis of mammalian complex IV inhibition by steroids. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	8
2956	Exploration of DNA processing features unravels novel properties of ICE conjugation in Gram-positive bacteria. <i>Nucleic Acids Research</i> , 2022, 50, 8127-8142.	6.5	1
2957	Decreased Interfacial Dynamics Caused by the N501Y Mutation in the SARS-CoV-2 S1 Spike:ACE2 Complex. <i>Frontiers in Molecular Biosciences</i> , 0, 9, .	1.6	9
2958	Structure-Function Relationships in Temperature Effects on Bacterial Luciferases: Nothing Is Perfect. <i>International Journal of Molecular Sciences</i> , 2022, 23, 8119.	1.8	2
2959	Development of Fenofibrate/Randomly Methylated β -Cyclodextrin-Loaded Eudragit® RL 100 Nanoparticles for Ocular Delivery. <i>Molecules</i> , 2022, 27, 4755.	1.7	9
2960	A Comparative Molecular Dynamics Study of Selected Point Mutations in the Shwachman-Bodian-Diamond Syndrome Protein SBDS. <i>International Journal of Molecular Sciences</i> , 2022, 23, 7938.	1.8	1
2961	Effect of Surface Hydrophobicity on the Adsorption of a Pilus-Derived Adhesin-like Peptide. <i>Langmuir</i> , 2022, 38, 9257-9265.	1.6	6
2962	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> , 2022, 18, 5025-5045.	2.3	5
2963	Molecular Dynamics of Enzyme-Substrate Complexes in Guanosine Trifosphate-Binding Proteins. <i>Russian Journal of Physical Chemistry B</i> , 2022, 16, 455-460.	0.2	4

#	ARTICLE	IF	CITATIONS
2964	Î²-Hydroxylation of Î±-amino-Î²-hydroxybutanoyl-glycyluridine catalyzed by a nonheme hydroxylase ensures the maturation of caprazamycin. <i>Communications Chemistry</i> , 2022, 5, .	2.0	2
2965	Conformational Dynamics and Mechanisms of Client Protein Integration into the Hsp90 Chaperone Controlled by Allosteric Interactions of Regulatory Switches: Perturbation-Based Network Approach for Mutational Profiling of the Hsp90 Binding and Allostery. <i>Journal of Physical Chemistry B</i> , 2022, 126, 5421-5442.	1.2	2
2966	Design of Peptides that Fold and Self-Assemble on Graphite. <i>Journal of Chemical Information and Modeling</i> , 0, , .	2.5	3
2967	A Multistage In Silico Study of Natural Potential Inhibitors Targeting SARS-CoV-2 Main Protease. <i>International Journal of Molecular Sciences</i> , 2022, 23, 8407.	1.8	36
2968	Ca ²⁺ -dependent interactions between lipids and the tumor-targeting peptide pHLIP. <i>Protein Science</i> , 2022, 31, .	3.1	8
2969	Structure and engineering of the minimal type VI CRISPR-Cas13bt3. <i>Molecular Cell</i> , 2022, 82, 3178-3192.e5.	4.5	12
2970	New quinoline and isatin derivatives as apoptotic VEGFR-2 inhibitors: design, synthesis, anti-proliferative activity, docking, ADMET, toxicity, and MD simulation studies. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2022, 37, 2191-2205.	2.5	35
2971	Origin of Protein Quake: Energy Waves Conducted by a Precise Mechanical Machine. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 5692-5702.	2.3	1
2972	On the Rapid Calculation of Binding Affinities for Antigen and Antibody Design and Affinity Maturation Simulations. <i>Antibodies</i> , 2022, 11, 51.	1.2	4
2973	Enzyme kinetics by <sc>GH7</sc> cellobiohydrolases on chromogenic substrates is dictated by non-productive binding: insights from crystal structures and <sc>MD</sc> simulation. <i>FEBS Journal</i> , 2023, 290, 379-399.	2.2	3
2974	Intermediates in SARS-CoV-2 spike-mediated cell entry. <i>Science Advances</i> , 2022, 8, .	4.7	24
2975	Construction of a Deep Neural Network Energy Function for Protein Physics. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 5649-5658.	2.3	5
2976	Peroxy Intermediate Drives Carbon Bond Activation in the Dioxygenase AsqJ. <i>Journal of the American Chemical Society</i> , 0, , .	6.6	3
2977	Cannabidivarin alleviates neuroinflammation by targeting TLR4 co-receptor MD2 and improves morphine-mediated analgesia. <i>Frontiers in Immunology</i> , 0, 13, .	2.2	2
2978	Amphiphilic Nanointerface: Inducing the Interfacial Activation for Lipase. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 39622-39636.	4.0	6
2980	Efficient synthesis 1,4-cyclohexanedicarboxaldehyde by an engineered alcohol oxidase. <i>Bioresources and Bioprocessing</i> , 2022, 9, .	2.0	0
2981	Preserving the Integrity of Empirical Force Fields. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3825-3831.	2.5	5
2982	Isolation and In Silico Inhibitory Potential against SARS-CoV-2 RNA Polymerase of the Rare Kaempferol 3-O-(6-O-acetyl)-Glucoside from <i>Calligonum tetrapterum</i> . <i>Plants</i> , 2022, 11, 2072.	1.6	10

#	ARTICLE	IF	CITATIONS
2983	Long-Time Oxygen Localization in Electron Transfer Flavoprotein. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 4191-4199.	2.5	5
2984	EML2-S constitutes a new class of proteins that recognizes and regulates the dynamics of tyrosinated microtubules. <i>Current Biology</i> , 2022, 32, 3898-3910.e14.	1.8	6
2985	A Uniquely Stable Trimeric Model of SARS-CoV-2 Spike Transmembrane Domain. <i>International Journal of Molecular Sciences</i> , 2022, 23, 9221.	1.8	1
2986	Multistep orthophosphate release tunes actomyosin energy transduction. <i>Nature Communications</i> , 2022, 13, .	5.8	21
2987	Structure of SARS-CoV-2 membrane protein essential for virus assembly. <i>Nature Communications</i> , 2022, 13, .	5.8	70
2989	Endogenous ligand recognition and structural transition of a human PTH receptor. <i>Molecular Cell</i> , 2022, 82, 3468-3483.e5.	4.5	28
2991	<scp>ppdx</scp>: Automated modeling of proteinâ€“protein interaction descriptors for use with machine learning. <i>Journal of Computational Chemistry</i> , 2022, 43, 1747-1757.	1.5	3
2992	Identification of a Thyroid Hormone Binding Site in Hsp90 with Implications for Its Interaction with Thyroid Hormone Receptor Beta. <i>ACS Omega</i> , 2022, 7, 28932-28945.	1.6	1
2993	Stabilization of Carbon Nanotubes and Graphene by Tween-80: Mechanistic Insights from Spectroscopic and Simulation Studies. <i>Langmuir</i> , 2022, 38, 10173-10182.	1.6	1
2994	Selfâ€“assembling Peptides with Internal Ionizable Unnatural Amino Acids: A General Approach to pHâ€“responsive Peptide Materials. <i>Chemistry - an Asian Journal</i> , 2022, 17, .	1.7	2
2996	Exploring the Dynamics of Shikimate Kinase through Molecular Mechanics. <i>Biophysica</i> , 2022, 2, 194-202.	0.6	1
2997	A Computational Study on the Interaction of NSP10 and NSP14: Unraveling the RNA Synthesis Proofreading Mechanism in SARS-CoV-2, SARS-CoV, and MERS-CoV. <i>ACS Omega</i> , 2022, 7, 29995-30014.	1.6	6
2998	Amino acid deprotonation rates from classical force fields. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	2
2999	SARS-CoV-2 Viroporins: A Multi-Omics Insight from Nucleotides to Amino Acids. <i>Applied Microbiology</i> , 2022, 2, 572-593.	0.7	1
3000	Structure-Based Virtual Screening, Docking, ADMET, Molecular Dynamics, and MM-PBSA Calculations for the Discovery of Potential Natural SARS-CoV-2 Helicase Inhibitors from the Traditional Chinese Medicine. <i>Journal of Chemistry</i> , 2022, 2022, 1-23.	0.9	9
3001	Mutual information analysis of mutation, nonlinearity, and triple interactions in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2023, 91, 121-133.	1.5	2
3002	Identifying ligand-binding specificity of the oligopeptide receptor OppA from <i>Bifidobacterium longum</i> KACC91563 by structure-based molecular modeling. <i>Arabian Journal of Chemistry</i> , 2022, , 104198.	2.3	0
3003	Tunnel connects lipid bilayer to occluded odorant-binding site of insect olfactory receptor. <i>Biophysical Chemistry</i> , 2022, 289, 106862.	1.5	4

#	ARTICLE	IF	CITATIONS
3004	Impact of arginine modified SNARE peptides on interactions with phospholipid bilayers and coiled-coil formation: A molecular dynamics study. <i>Journal of Molecular Liquids</i> , 2022, 364, 119972.	2.3	0
3005	Interaction of Lassa virus fusion and membrane proximal peptides with late endosomal membranes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2022, 1864, 184031.	1.4	1
3006	Omicron BA.1 and BA.2 variants increase the interactions of SARS-CoV-2 spike glycoprotein with ACE2. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 117, 108286.	1.3	20
3007	A quantitative study of the structure-activity relationship and molecular docking of 5.6.7-trimethoxy-N-aryl-2-styrylquinolin-4-amines as potential anticancer agents using quantum chemical descriptors and statistical methods. <i>Journal of Molecular Structure</i> , 2022, 1270, 133794.	1.8	5
3008	Identification of Drug Combination Therapies for SARS-CoV-2: A Molecular Dynamics Simulations Approach. <i>Drug Design, Development and Therapy</i> , 0, Volume 16, 2995-3013.	2.0	6
3010	Molecular dynamics simulations highlight the altered binding landscape at the spike-ACE2 interface between the Delta and Omicron variants compared to the SARS-CoV-2 original strain. <i>Computers in Biology and Medicine</i> , 2022, 149, 106035.	3.9	14
3011	Pharmacogenetics of human sulfotransferases and impact of amino acid exchange on Phase II drug metabolism. <i>Drug Discovery Today</i> , 2022, 27, 103349.	3.2	17
3012	Insighting the inhibitory potential of novel modafinil drug derivatives against estrogen alpha (ER α) of breast cancer through a triple hybrid computational methodology. <i>Journal of Molecular Liquids</i> , 2022, 366, 120234.	2.3	17
3013	Characterization of adjacent charged residues near the agonist binding site of the nematode UNC-49 GABA receptor. <i>Molecular and Biochemical Parasitology</i> , 2022, 252, 111521.	0.5	1
3014	Distinct mode of membrane interaction and disintegration by diverse class of antimicrobial peptides. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2022, 1864, 184047.	1.4	2
3015	A mechanistic investigation on kokumi-active β -Glutamyl tripeptides – A computational study to understand molecular basis of their activity and to identify novel potential kokumi-tasting sequences. <i>Food Research International</i> , 2022, 162, 111932.	2.9	10
3016	Molecular dynamics. , 2023, , 431-443.		1
3017	Planning, executing and assessing the validity of SANS contrast variation experiments. <i>Methods in Enzymology</i> , 2022, , .	0.4	0
3018	Molecular dynamics analysis of biomolecular systems including nucleic acids. <i>Biophysics and Physicobiology</i> , 2022, 19, n/a.	0.5	2
3019	Crystal structure prediction of host-guest supramolecular systems based on β -cyclodextrin dimers and trimers with luminescent probes. <i>CrystEngComm</i> , 2022, 24, 6654-6661.	1.3	1
3020	Computational study of quinoline-based thiadiazole compounds as potential antileishmanial inhibitors. <i>New Journal of Chemistry</i> , 2022, 46, 17554-17576.	1.4	9
3021	Computational modeling of potential milciclib derivatives inhibitor-CDK2 binding through global docking and accelerated molecular dynamics simulations. <i>Informatics in Medicine Unlocked</i> , 2022, 33, 101069.	1.9	4
3022	Long-Timescale Simulations Revealed Critical Non-Conserved Residues of Phosphodiesterases Affecting Selectivity of BAY60-7550. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 5136-5149.	1.9	0

#	ARTICLE	IF	CITATIONS
3023	Molecular Modeling Studies of Natural Inhibitors of Androgen Signaling in Prostate Cancer. <i>Cancer Informatics</i> , 2022, 21, 117693512211185.	0.9	8
3024	Mechanistic Insights into Structural Stability of the Selectivity Filters in Typical Cation Channels. <i>Journal of Materials Science and Chemical Engineering</i> , 2022, 10, 17-32.	0.2	0
3025	Effect of a monovalent salt on the energetics of an antimicrobial-peptide: micelle dissociation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 23669-23678.	1.3	1
3026	Molecular dynamics analysis of the structural properties of the transglutaminases of <i>Kutzneria albida</i> and <i>Streptomyces mobaraensis</i> . <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 3924-3934.	1.9	3
3027	Computer-aided drug design applied to a series of pyridinyl imidazole derivatives targeting p38 \hat{I} MAP kinase: 2D-QSAR, docking, MD simulation, and ADMET investigations. <i>New Journal of Chemistry</i> , 2022, 46, 20786-20800.	1.4	4
3028	End-to-end differentiable construction of molecular mechanics force fields. <i>Chemical Science</i> , 2022, 13, 12016-12033.	3.7	17
3029	Computational Assessment of Xanthones from African Medicinal Plants as Aldose Reductase Inhibitors. <i>Computation</i> , 2022, 10, 146.	1.0	5
3030	Multi-spectroscopic, thermodynamic, and molecular docking/dynamic approaches for characterization of the binding interaction between calf thymus DNA and palbociclib. <i>Scientific Reports</i> , 2022, 12, .	1.6	9
3031	Studying folding \rightarrow unfolding dynamics of solvated alanine polypeptides using molecular dynamics. <i>European Physical Journal D</i> , 2022, 76, .	0.6	1
3032	Information Transfer in Active States of Human $\hat{I}2$ -Adrenergic Receptor via Inter-Rotameric Motions of Loop Regions. <i>Applied Sciences (Switzerland)</i> , 2022, 12, 8530.	1.3	2
3033	Structural basis of ion uptake in copper-transporting P1B-type ATPases. <i>Nature Communications</i> , 2022, 13, .	5.8	6
3034	Applications of Molecular Dynamics Simulation in Protein Study. <i>Membranes</i> , 2022, 12, 844.	1.4	18
3036	MDO: A Computational Protocol for Prediction of Flexible Enzyme-Ligand Binding Mode. <i>Current Computer-Aided Drug Design</i> , 2022, 18, .	0.8	0
3038	Electric fields control water-gated proton transfer in cytochrome <i>c</i> oxidase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	10
3040	In silico study on the Hepatitis E virus RNA Helicase and its inhibition by silvestrol, rocaglamide and other flavagline compounds. <i>Scientific Reports</i> , 2022, 12, .	1.6	2
3041	Parametrization of Force Field Bonded Terms under Structural Inconsistency. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 4771-4782.	2.5	0
3042	Modified Protein-Water Interactions in CHARMM36m for Thermodynamics and Kinetics of Proteins in Dilute and Crowded Solutions. <i>Molecules</i> , 2022, 27, 5726.	1.7	5
3043	Engineering SARS-CoV-2 specific cocktail antibodies into a bispecific format improves neutralizing potency and breadth. <i>Nature Communications</i> , 2022, 13, .	5.8	16

#	ARTICLE	IF	CITATIONS
3044	Fisetin induces apoptosis in human skin cancer cells through downregulating MTH1. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 7339-7353.	2.0	4
3045	Gene expression profile analysis unravelled the systems level association of renal cell carcinoma with diabetic nephropathy and Matrix-metalloproteinase-9 as a potential therapeutic target. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 7535-7550.	2.0	0
3046	Importance of molecular dynamics equilibrium protocol on protein-lipid interaction near channel pore. <i>Biophysical Reports</i> , 2022, 2, 100080.	0.7	4
3047	Intermolecular Interactions of Nucleoside Antibiotic Tunicamycin with On-Target MraY_{CB}-TUN and Off-Target DPAGT1-TUN in the Active Sites Delineated by Quantum Mechanics/Molecular Mechanics Calculations. <i>ACS Omega</i> , 2022, 7, 32970-32987.	1.6	2
3048	Best Practices in Constant pH MD Simulations: Accuracy and Sampling. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 6134-6147.	2.3	14
3049	Identification of promising anti-EBOV inhibitors: <i>de novo</i> drug design, molecular docking and molecular dynamics studies. <i>Royal Society Open Science</i> , 2022, 9, .	1.1	3
3050	Accurate p <i>K</i> _a Calculations in Proteins with Reactive Molecular Dynamics Provide Physical Insight Into the Electrostatic Origins of Their Values. <i>Journal of Physical Chemistry B</i> , 2022, 126, 7321-7330.	1.2	2
3051	Galvani Offset Potential and Constant-pH Simulations of Membrane Proteins. <i>Journal of Physical Chemistry B</i> , 2022, 126, 6868-6877.	1.2	13
3052	Self-Uptake Mechanism of Polymyxin-Based Lipopeptide against Gram-Negative Bacterial Membrane: Role of the First Adsorbed Lipopeptide. <i>Journal of Physical Chemistry B</i> , 2022, 126, 8222-8232.	1.2	2
3053	Sibling rivalry among the ZBTB transcription factor family: homodimers versus heterodimers. <i>Life Science Alliance</i> , 2022, 5, e202201474.	1.3	3
3054	Native and activated antithrombin inhibits TMPRSS2 activity and SARS-CoV-2 infection. <i>Journal of Medical Virology</i> , 2023, 95, .	2.5	13
3055	Bell-Evans model and steered molecular dynamics in uncovering the dissociation kinetics of ligands targeting G-protein-coupled receptors. <i>Scientific Reports</i> , 2022, 12, .	1.6	4
3056	Medium-Chain Lipid Conjugation Facilitates Cell-Permeability and Bioactivity. <i>Journal of the American Chemical Society</i> , 2022, 144, 18532-18544.	6.6	23
3057	Role of TM3 in claudin-15 strand flexibility: A molecular dynamics study. <i>Frontiers in Molecular Biosciences</i> , 0, 9, .	1.6	6
3059	Immunoinformatics Approach to Design Novel Subunit Vaccine against the Epstein-Barr Virus. <i>Microbiology Spectrum</i> , 2022, 10, .	1.2	10
3060	In Silico Conformational Features of Botulinum Toxins A1 and E1 According to Intraluminal Acidification. <i>Toxins</i> , 2022, 14, 644.	1.5	2
3061	Thermostabilizing mechanisms of canonical single amino acid substitutions at a <sc>GH1</sc> Î±-glucosidase probed by multiple <sc>MD</sc> and computational approaches. <i>Proteins: Structure, Function and Bioinformatics</i> , 2023, 91, 218-236.	1.5	2
3062	Single-chain insulin analogs threaded by the insulin receptor Î±CT domain. <i>Biophysical Journal</i> , 2022, 121, 4063-4077.	0.2	2

#	ARTICLE	IF	CITATIONS
3064	Multiple conserved states characterize the twist landscape of the bacterial actin homolog MreB. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 5838-5846.	1.9	0
3065	Discovery of Small Molecule Agonist of Gonadotropin-Releasing Hormone Receptor (GnRH1R). <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 5009-5022.	2.5	4
3068	General Design Strategy to Precisely Control the Emission of Fluorophores via a Twisted Intramolecular Charge Transfer (TICT) Process. <i>Journal of the American Chemical Society</i> , 2022, 144, 19778-19790.	6.6	41
3069	Modeling, energetic and structural analysis of peptide membranes formed by arginine and phenylalanine (R2F4R2) using fully atomistic molecular dynamics. <i>Journal of Molecular Liquids</i> , 2022, 367, 120498.	2.3	1
3070	Biological effect of black phosphorus nanosheets on the interaction between SARS-CoV-2 S protein and ACE2. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 27388-27393.	1.3	1
3071	Cardiolipin, and not monolysocardiolipin, preferentially binds to the interface of complexes III and IV. <i>Chemical Science</i> , 2022, 13, 13489-13498.	3.7	3
3072	Extremophilic behavior of catalytic amyloids sustained by backbone structuring. <i>Journal of Materials Chemistry B</i> , 2022, 10, 9400-9412.	2.9	1
3073	Multiscale modelling of claudin-based assemblies: A magnifying glass for novel structures of biological interfaces. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 5984-6010.	1.9	5
3074	Programming xenon diffusion in maltose-binding protein. <i>Biophysical Journal</i> , 2022, 121, 4635-4643.	0.2	4
3075	Structural insights into light-driven anion pumping in cyanobacteria. <i>Nature Communications</i> , 2022, 13, .	5.8	4
3076	Structure of the human heterodimeric transporter 4F2hc-LAT2 in complex with Anticalin, an alternative binding protein for applications in single-particle cryo-EM. <i>Scientific Reports</i> , 2022, 12, .	1.6	3
3077	Structure and Computational Electrophysiology of Ac-LS3, a Synthetic Ion Channel. <i>Journal of Physical Chemistry B</i> , 2022, 126, 8985-8999.	1.2	1
3078	Influence of the Active Site Flexibility on the Efficiency of Substrate Activation in the Active Sites of Bi-Zinc Metallo- β -Lactamases. <i>Molecules</i> , 2022, 27, 7031.	1.7	1
3079	Inhibited KdpFABC transitions into an E1 off-cycle state. <i>ELife</i> , 0, 11, .	2.8	5
3080	Lateral fenestrations in the extracellular domain of the glycine receptor contribute to the main chloride permeation pathway. <i>Science Advances</i> , 2022, 8, .	4.7	2
3081	Engineered helicase replaces thermocycler in DNA amplification while retaining desired PCR characteristics. <i>Nature Communications</i> , 2022, 13, .	5.8	10
3082	Crystal structure of the Na ⁺ /H ⁺ antiporter NhaA at active pH reveals the mechanistic basis for pH sensing. <i>Nature Communications</i> , 2022, 13, .	5.8	14
3084	Activation mechanism of the mouse cold-sensing TRPM8 channel by cooling agonist and PIP ₂ . <i>Science</i> , 2022, 378, .	6.0	22

#	ARTICLE	IF	CITATIONS
3086	Structural insights into adhesion GPCR ADGRL3 activation and Gq, Gs, Gi, and G12 coupling. <i>Molecular Cell</i> , 2022, 82, 4340-4352.e6.	4.5	18
3087	On the energetic differences of avian cryptochromes 4 from selected species. <i>European Physical Journal D</i> , 2022, 76, .	0.6	5
3088	Modulation of Diffusion Mechanism and Its Correlation with Complexation in Aqueous Deep Eutectic Solvents. <i>Journal of Physical Chemistry B</i> , 2022, 126, 9026-9037.	1.2	2
3090	Quantum-based modeling of protein-ligand interaction: The complex of RutA with uracil and molecular oxygen. <i>Molecular Informatics</i> , 0, , .	1.4	1
3091	Characterizing Transient Protein-Protein Interactions by Trp-Cys Quenching and Computer Simulations. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 10175-10182.	2.1	0
3092	In vitro and in silico characteristics of doxorubicin-loaded four polymeric-based polysaccharides-modified super paramagnetic iron oxide nanoparticles for cancer chemotherapy and magnetic resonance imaging. <i>International Journal of Polymeric Materials and Polymeric Biomaterials</i> , 0, , 1-14.	1.8	0
3093	An N-glycan on the C2 domain of JAGGED1 is important for Notch activation. <i>Science Signaling</i> , 2022, 15, .	1.6	3
3094	Ion transfer mechanisms in Mrp-type antiporters from high resolution cryoEM and molecular dynamics simulations. <i>Nature Communications</i> , 2022, 13, .	5.8	6
3095	Effect of Viscous Media on the Photophysical Characteristics of Flavin Mononucleotide. <i>Bulletin of the Russian Academy of Sciences: Physics</i> , 2022, 86, 1196-1202.	0.1	1
3096	Mechanism of 4-aminopyridine inhibition of the lysosomal channel TMEM175. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	6
3097	Structural Achievability of an NH ⁺ ⋯ ⁻ Interaction between Gln and Phe in a Crystal Structure of a Collagen-like Peptide. <i>Biomolecules</i> , 2022, 12, 1433.	1.8	5
3098	Designing an Epitope-Based Peptide Vaccine Derived from RNA-Dependent RNA Polymerase (RdRp) against Dengue Virus Serotype 2. <i>Vaccines</i> , 2022, 10, 1734.	2.1	2
3099	Probing Methyl Group Dynamics in Proteins by NMR Cross-Correlated Dipolar Relaxation and Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 7722-7732.	2.3	6
3100	Molecular mechanism of claudin-15 strand flexibility: A computational study. <i>Journal of General Physiology</i> , 2022, 154, .	0.9	10
3102	Targeted regulation of pulsed electric field (PEF) treatment on responsive amino acids based on the molecular dynamic simulation. <i>Innovative Food Science and Emerging Technologies</i> , 2022, 82, 103197.	2.7	4
3103	EF4K bola-amphiphilic peptide nanomembrane: structural, energetic and dynamic properties using molecular dynamics. <i>Journal of Molecular Liquids</i> , 2022, 368, 120651.	2.3	1
3104	Explicit-solute implicit-solvent molecular simulation with binary level-set, adaptive-mobility, and GPU. <i>Journal of Computational Physics</i> , 2023, 472, 111673.	1.9	0
3107	Influence of Selective Extraction/Isolation of Heme/Hemoglobin with Hydrophobic Imidazolium Ionic Liquids on the Precision and Accuracy of Cotinine ELISA Test. <i>International Journal of Molecular Sciences</i> , 2022, 23, 13692.	1.8	0

#	ARTICLE	IF	CITATIONS
3108	The Discovery of Potential SARS-CoV-2 Natural Inhibitors among 4924 African Metabolites Targeting the Papain-like Protease: A Multi-Phase In Silico Approach. <i>Metabolites</i> , 2022, 12, 1122.	1.3	3
3109	Ingenuity in performing replica permutation: How to order the state labels for improving sampling efficiency. <i>Journal of Computational Chemistry</i> , 2023, 44, 534-545.	1.5	5
3110	Linear One-Dimensional Assembly of Metal Nanostructures onto an Asymmetric Peptide Nanofiber with High Persistence Length. <i>ACS Nano</i> , 2022, 16, 18307-18314.	7.3	1
3111	Structural and energetic analyses of SARS-CoV-2 N-terminal domain characterise sugar binding pockets and suggest putative impacts of variants on COVID-19 transmission. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 6302-6316.	1.9	0
3112	Mechanical Unfolding and Refolding of NanoLuc via Single-Molecule Force Spectroscopy and Computer Simulations. <i>Biomacromolecules</i> , 2022, 23, 5164-5178.	2.6	1
3113	Atomistic Pictures of Self-Assembled Helical Peptide Nanofibers. <i>Journal of Physical Chemistry B</i> , 2022, 126, 9476-9492.	1.2	0
3114	Investigation of the halophilic PET hydrolase PET6 from <i>Vibrio gazogenes</i> . <i>Protein Science</i> , 2022, 31, .	3.1	8
3115	Molecular Dynamics Simulation for Investigating Antigen-Antibody Interaction. <i>Methods in Molecular Biology</i> , 2023, , 101-107.	0.4	1
3116	GPU-Accelerated All-Atom Particle-Mesh Ewald Continuous Constant pH Molecular Dynamics in Amber. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 7510-7527.	2.3	19
3117	An active site loop toggles between conformations to control antibiotic hydrolysis and inhibition potency for CTX-M β -lactamase drug-resistance enzymes. <i>Nature Communications</i> , 2022, 13, .	5.8	3
3120	A Computer Simulation Insight into the Formation of Apocarotenoids: Study of the Carotenoid Oxygenases BCO1 and BCO2 and Their Interaction with Putative Substrates. <i>Molecules</i> , 2022, 27, 7813.	1.7	0
3121	Structural analysis of a simplified model reproducing SARS-CoV-2 S RBD/ACE2 binding site. <i>Heliyon</i> , 2022, 8, e11568.	1.4	4
3122	Capturing the Polarization Response of Solvated Proteins under Constant Electric Fields in Molecular Dynamics Simulations. <i>ChemPhysChem</i> , 2023, 24, .	1.0	1
3123	Inter-Site Cooperativity of Calmodulin N-Terminal Domain and Phosphorylation Synergistically Improve the Affinity and Selectivity for Uranyl. <i>Biomolecules</i> , 2022, 12, 1703.	1.8	2
3124	Molecular origins of asymmetric proton conduction in the influenza M2 channel. <i>Biophysical Journal</i> , 2023, 122, 90-98.	0.2	2
3125	A novel insight into the binding behavior between soy protein and homologous ketones: Perspective from steric effect. <i>Journal of Molecular Liquids</i> , 2023, 369, 120895.	2.3	5
3126	Unveiling the structural features that regulate carbapenem deacylation in KPC-2 through QM/MM and interpretable machine learning. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 1349-1362.	1.3	2
3127	Development of the force field for cyclosporine A. <i>Biophysics and Physicobiology</i> , 2022, 19, n/a.	0.5	0

#	ARTICLE	IF	CITATIONS
3128	How Do Salt and Lipids Affect Conformational Dynamics of A β 42 Monomers in Water?. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	3
3130	The Mechanism of Selective Recognition of Lipid Substrate by hDHC20 Enzyme. <i>International Journal of Molecular Sciences</i> , 2022, 23, 14791.	1.8	1
3131	Perfluoroalkyl substances (PFASs) are substrates of the renal human organic anion transporter 4 (OAT4). <i>Archives of Toxicology</i> , 2023, 97, 685-696.	1.9	8
3133	Computer-Aided Drug Design: An Update. <i>Methods in Molecular Biology</i> , 2023, , 123-152.	0.4	5
3134	A Simplified Treatment for Efficiently Modeling the Spectral Signal of Vibronic Transitions: Application to Aqueous Indole. <i>Molecules</i> , 2022, 27, 8135.	1.7	3
3135	Mechanism of chemical reactions in the active site of aspartate N-acetyltransferase NAT8L revealed by molecular modeling. <i>Mendeleev Communications</i> , 2022, 32, 739-741.	0.6	6
3136	Molecular mechanism of drug transport and release through zeolitic imidazole framework nanospheres for versatile drug delivery applications. <i>Journal of Molecular Liquids</i> , 2023, 371, 120822.	2.3	2
3137	SARS-CoV-2 Delta Variant: Interplay between Individual Mutations and Their Allosteric Synergy. <i>Biomolecules</i> , 2022, 12, 1742.	1.8	6
3138	Physiological changes in bilayer thickness induced by cholesterol control GPCR rhodopsin function. <i>Biophysical Journal</i> , 2023, 122, 973-983.	0.2	8
3139	In Silico Studies to Predict the Role of Solvent in Guiding the Conformations of Intrinsically Disordered Peptides and Their Aggregated Protofilaments. <i>ACS Omega</i> , 2022, 7, 43337-43345.	1.6	0
3140	Glycoprotein attachment with host cell surface receptor ephrin B2 and B3 in mediating entry of nipah and hendra virus: a computational investigation. <i>Journal of Chemical Sciences</i> , 2022, 134, .	0.7	5
3141	Inhibition of mutant RAS-RAF interaction by mimicking structural and dynamic properties of phosphorylated RAS. <i>ELife</i> , 0, 11, .	2.8	4
3142	Enthalpic and entropic contributions to the activation free energy of single noncovalent bonds in molecular systems: A computational methodology. <i>Physical Review A</i> , 2022, 106, .	1.0	1
3143	Quantitative Predictions and Experimental Validation of Liquid-Vapor Interfacial Tension in Binary and Ternary Mixtures of Alkanes Using Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2023, 127, 396-406.	1.2	0
3144	Design, Synthesis and Assay of Novel Methylxanthine-Alkynylmethylamine Derivatives as Acetylcholinesterase Inhibitors. <i>Molecules</i> , 2022, 27, 8787.	1.7	3
3145	Evolution of Ceftriaxone Resistance of Penicillin-Binding Proteins 2 Revealed by Molecular Modeling. <i>International Journal of Molecular Sciences</i> , 2023, 24, 176.	1.8	0
3146	CryoEM structures of anion exchanger 1 capture multiple states of inward- and outward-facing conformations. <i>Communications Biology</i> , 2022, 5, .	2.0	10
3147	Nirmatrelvir-resistant SARS-CoV-2 variants with high fitness in an infectious cell culture system. <i>Science Advances</i> , 2022, 8, .	4.7	90

#	ARTICLE	IF	CITATIONS
3148	Insights into autoregulation of a membrane protein complex by its cytoplasmic domains. <i>Biophysical Journal</i> , 2023, 122, 577-594.	0.2	1
3150	Amyotrophic lateral sclerosis disease-related mutations disrupt the dimerization of superoxide dismutase 1 - A comparative molecular dynamics simulation study. <i>Computers in Biology and Medicine</i> , 2022, 151, 106319.	3.9	4
3151	A comparative quantitative structural assessment of benzothiazine-derived HDAC8 inhibitors by predictive ligand-based drug designing approaches. <i>SAR and QSAR in Environmental Research</i> , 2022, 33, 987-1011.	1.0	3
3152	An In-Silico Evaluation of Anthraquinones as Potential Inhibitors of DNA Gyrase B of <i>Mycobacterium tuberculosis</i> . <i>Microorganisms</i> , 2022, 10, 2434.	1.6	5
3154	A Chimeric Peptide Inhibits Red Blood Cell Invasion by <i>Plasmodium falciparum</i> with Hundredfold Increased Efficacy**. <i>ChemBioChem</i> , 2023, 24, .	1.3	1
3155	Molecular dynamics studies of CED ⁴ /CED ⁹ /EGL ¹ ternary complex reveal CED ⁴ release mechanism in the linear apoptotic pathway of <i>Caenorhabditis elegans</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2023, 91, 679-693.	1.5	0
3159	Allosteric regulation in STAT3 interdomains is mediated by a rigid core: SH2 domain regulation by CCD in D170A variant. <i>PLoS Computational Biology</i> , 2022, 18, e1010794.	1.5	1
3161	The Role of the Extrafibrillar Volume on the Mechanical Properties of Molecular Models of Mineralized Bone Microfibrils. <i>ACS Biomaterials Science and Engineering</i> , 2023, 9, 230-245.	2.6	2
3162	ADMET prediction, Docking, DM analysis and antibacterial screening of epoxy furan-clerodanes from <i>Croton hypoleucus</i> . <i>Journal of Molecular Structure</i> , 2023, 1277, 134840.	1.8	3
3165	Small GTPase Ran: Depicting the nucleotide-specific conformational landscape of the functionally important C-terminus. <i>Frontiers in Molecular Biosciences</i> , 0, 10, .	1.6	0
3166	Comparative Study of Receptor-, Receptor State-, and Membrane-Dependent Cholesterol Binding Sites in A _{2A} and A ₁ Adenosine Receptors Using Coarse-Grained Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 928-949.	2.5	5
3168	Network Hamiltonian Models for Unstructured Protein Aggregates, with Application to ¹³ D-Crystallin. <i>Journal of Physical Chemistry B</i> , 2023, 127, 685-697.	1.2	2
3170	Cryo-EM structures of orphan GPR21 signaling complexes. <i>Nature Communications</i> , 2023, 14, .	5.8	9
3171	Bergamottin: location, aggregation and interaction with the plasma membrane. <i>Journal of Biomolecular Structure and Dynamics</i> , 0, , 1-12.	2.0	1
3172	Towards <i>de novo</i> design of transmembrane α -helical assemblies using structural modelling and molecular dynamics simulation. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 3595-3606.	1.3	2
3174	Effect of Salts on the Conformational Dynamics of the Cytochrome P450 OleP. <i>Molecules</i> , 2023, 28, 832.	1.7	0
3175	Multiscale molecular dynamics simulations predict arachidonic acid binding sites in human ASIC1a and ASIC3 transmembrane domains. <i>Journal of General Physiology</i> , 2023, 155, .	0.9	1
3176	Xanthatin and 8-epi-xanthatin as new potential colchicine binding site inhibitors: a computational study. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	0

#	ARTICLE	IF	CITATIONS
3177	Conformational and mechanical stability of the isolated large subunit of membrane-bound [NiFe]-hydrogenase from <i>Cupriavidus necator</i> . <i>Frontiers in Microbiology</i> , 0, 13, .	1.5	1
3178	Extracellular Fe(III) reductase structure reveals a modular organization enabling S-layer insertion and electron transfer to insoluble substrates. <i>Structure</i> , 2023, 31, 174-184.e3.	1.6	0
3179	Modeling Light-Induced Chromophore Hydration in the Reversibly Photoswitchable Fluorescent Protein Dreiklang. <i>Molecules</i> , 2023, 28, 505.	1.7	2
3180	Revisiting autoimmune lymphoproliferative syndrome caused by Fas ligand mutations. <i>Journal of Allergy and Clinical Immunology</i> , 2023, 151, 1391-1401.e7.	1.5	5
3181	LongBondEliminator: A Molecular Simulation Tool to Remove Ring Penetrations in Biomolecular Simulation Systems. <i>Biomolecules</i> , 2023, 13, 107.	1.8	1
3182	Discovery of new quinoline and isatine derivatives as potential VEGFR-2 inhibitors: design, synthesis, antiproliferative, docking and MD simulation studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 11535-11550.	2.0	6
3183	Ensemble-based, high-throughput virtual screening of potential inhibitor targeting putative farnesol dehydrogenase of <i>Metisa plana</i> (Lepidoptera: Psychidae). <i>Computational Biology and Chemistry</i> , 2023, 103, 107811.	1.1	2
3184	Effect of tryptophan mutation on the structure of LOV1 domain of phototropin1 protein of <i>Ostreococcus tauri</i> : A combined molecular dynamics simulation and biophysical approach. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2023, 1867, 130304.	1.1	2
3185	Development of hidden Markov modeling method for molecular orientations and structure estimation from high-speed atomic force microscopy time-series images. <i>PLoS Computational Biology</i> , 2022, 18, e1010384.	1.5	2
3187	Green-Solvent Engineering for Depositing Qualified Phenyl-C61-butyl Acid Methyl Ester Films for Inverted Flexible Perovskite Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 1042-1052.	4.0	2
3188	Probing ion binding in the selectivity filter of the Cav1.1 channel with molecular dynamics. <i>Biophysical Journal</i> , 2023, 122, 496-505.	0.2	1
3189	SARS-CoV-2 accessory proteins ORF7a and ORF3a use distinct mechanisms to down-regulate MHC-I surface expression. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2023, 120, .	3.3	49
3190	Identification and Characterization of ML321: A Novel and Highly Selective D ₂ Dopamine Receptor Antagonist with Efficacy in Animal Models That Predict Atypical Antipsychotic Activity. <i>ACS Pharmacology and Translational Science</i> , 2023, 6, 151-170.	2.5	1
3191	Structural correlations of nitrogenase active sites using nuclear resonance vibrational spectroscopy and QM/MM calculations. <i>Faraday Discussions</i> , 0, 243, 253-269.	1.6	1
3192	State-specific morphological deformations of the lipid bilayer explain mechanosensitive gating of MscS ion channels. <i>ELife</i> , 0, 12, .	2.8	10
3193	Resistance to a tyrosine kinase inhibitor mediated by changes to the conformation space of the kinase. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 6175-6183.	1.3	1
3194	Effect of substrate charge density on the adsorption of intrinsically disordered protein amyloid β 40: a molecular dynamics study. <i>Soft Matter</i> , 0, , .	1.2	0
3195	Impacts of external electric fields on the permeation of glycerol and water molecules through aquaglyceroporin-7: molecular dynamics simulation approach. <i>European Physical Journal E</i> , 2023, 46, .	0.7	0

#	ARTICLE	IF	CITATIONS
3196	Structure and supramolecular organization of the canine distemper virus attachment glycoprotein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2023, 120, .	3.3	7
3197	A Computational Inter-Species Study on Safrole Phase I Metabolism-Dependent Bioactivation: A Mechanistic Insight into the Study of Possible Differences among Species. <i>Toxins</i> , 2023, 15, 94.	1.5	3
3199	Molecular dynamics study of Cl ⁻ permeation through cystic fibrosis transmembrane conductance regulator (CFTR). <i>Cellular and Molecular Life Sciences</i> , 2023, 80, .	2.4	6
3200	Simulation of Complex Biomolecular Systems: The Ribosome Challenge. <i>Annual Review of Biophysics</i> , 2023, 52, 361-390.	4.5	2
3201	Identification of Novel CB2 Ligands through Virtual Screening and In Vitro Evaluation. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 1012-1027.	2.5	1
3202	Non-Equivalence of Monomers in the Dimeric Structure of a Bacterial Photoactivated Adenylyl Cyclase. <i>Biophysics (Russian Federation)</i> , 2022, 67, 895-901.	0.2	0
3203	Helical intermediate formation and its role in amyloids of an amphibian antimicrobial peptide. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 12134-12147.	1.3	2
3204	A hybrid approach for coarse-graining helical peptoids: Solvation, secondary structure, and assembly. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	4
3206	Improving Properties of Podophyllic Aldehyde-Derived Cyclolignans: Design, Synthesis and Evaluation of Novel Lignohydroquinones, Dual-Selective Hybrids against Colorectal Cancer Cells. <i>Pharmaceutics</i> , 2023, 15, 886.	2.0	2
3207	Partial Destabilization of Amyloid- β Protofibril by Methionine Photo-Oxidation: A Molecular Dynamic Simulation Study. <i>ACS Omega</i> , 2023, 8, 10148-10159.	1.6	1
3208	Computational Modeling of the Interaction of Molecular Oxygen with the miniSOG Protein—A Light Induced Source of Singlet Oxygen. <i>Biophysica</i> , 2023, 3, 252-262.	0.6	0
3209	Bridging Thermodynamics, Antimicrobial Activity, and pH Sensitivity of Cationic Membranolytic Heptapeptides—A Computational and Experimental Study. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 2393-2408.	2.5	2
3210	Constrained catecholamines gain β 2AR selectivity through allosteric effects on pocket dynamics. <i>Nature Communications</i> , 2023, 14, .	5.8	5
3211	The impact of pathogenic and artificial mutations on Claudin-5 selectivity from molecular dynamics simulations. <i>Computational and Structural Biotechnology Journal</i> , 2023, 21, 2640-2653.	1.9	2
3212	Engineering a membrane-binding protein to trimerize and induce high membrane curvature. <i>Biophysical Journal</i> , 2023, 122, 3008-3017.	0.2	1
3213	Engineering of conserved residues near antibody heavy chain complementary determining region 3 (HCDR3) improves both affinity and stability. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2023, 1871, 140915.	1.1	1
3214	Bioinformatics approaches to discovering food-derived bioactive peptides: Reviews and perspectives. <i>TrAC - Trends in Analytical Chemistry</i> , 2023, 162, 117051.	5.8	23
3215	Spectroscopic analysis, kinetic mechanism, computational docking, and molecular dynamics of active metabolites from the aerial parts of <i>Astragalus membranaceus</i> Bunge as tyrosinase inhibitors. <i>Bioorganic Chemistry</i> , 2023, 134, 106464.	2.0	3

#	ARTICLE	IF	CITATIONS
3216	GAP positions catalytic H-Ras residue Q61 for GTP hydrolysis in molecular dynamics simulations, complicating chemical rescue of Ras deactivation. <i>Computational Biology and Chemistry</i> , 2023, 104, 107835.	1.1	0
3217	Use of computational and wet lab techniques to examine the molecular association between a potent hepatitis C virus inhibitor, PSI-6206 and human serum albumin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2023, 294, 122543.	2.0	2
3218	Mechano-Redox Control of Mac-1 De-Adhesion by PDI Promotes Directional Movement Under Flow. <i>Circulation Research</i> , 2023, 132, .	2.0	5
3219	Influence of electronic polarization on the binding of anions to a chloride-pumping rhodopsin. <i>Biophysical Journal</i> , 2023, 122, 1548-1556.	0.2	2
3220	Resolving Protein Conformational Plasticity and Substrate Binding via Machine Learning. <i>Journal of Chemical Theory and Computation</i> , 0, , .	2.3	0
3221	Structural intrinsic disorder in a functionalized potyviral coat protein as a main viability determinant of its assembled nanoparticles. <i>International Journal of Biological Macromolecules</i> , 2023, 236, 123958.	3.6	2
3222	Molecular dynamics simulations of the calmodulin-induced $\hat{I}\pm$ -helix in the SK2 calcium-gated potassium ion channel. <i>Journal of Biological Chemistry</i> , 2023, 299, 102850.	1.6	0
3223	Atomistic insights on the adsorption of long-chain undecane molecules on carbon nanotubes: Roles of chirality and surface hydroxylation. <i>Diamond and Related Materials</i> , 2023, 133, 109706.	1.8	2
3224	The role of conformational change and key glutamic acid residues in the ClC-ec1 antiporter. <i>Biophysical Journal</i> , 2023, 122, 1068-1085.	0.2	1
3225	Identifying molecular targets of Aspiletrein-derived steroidal saponins in lung cancer using network pharmacology and molecular docking-based assessments. <i>Scientific Reports</i> , 2023, 13, .	1.6	7
3227	Universal QM/MM approaches for general nanoscale applications. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2023, 13, .	6.2	10
3229	Evidence That Less Can Be More for Transferable Force Fields. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 1188-1195.	2.5	0
3230	May the force be with you: The role of hyper-mechanostability of the bone sialoprotein binding protein during early stages of Staphylococci infections. <i>Frontiers in Chemistry</i> , 0, 11, .	1.8	2
3231	Structure-based virtual screening of novel natural products as chalcone derivatives against SARS-CoV-2 M ^{pro} . <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 13235-13249.	2.0	4
3232	Alizarin as a potential protector of proteins against damage caused by hydroperoxyl radical. <i>Chemico-Biological Interactions</i> , 2023, 373, 110395.	1.7	0
3233	Comparative Modeling and Analysis of Extremophilic D-Ala-D-Ala Carboxypeptidases. <i>Biomolecules</i> , 2023, 13, 328.	1.8	0
3235	Reversal of the unique Q493R mutation increases the affinity of Omicron S1-RBD for ACE2. <i>Computational and Structural Biotechnology Journal</i> , 2023, 21, 1966-1977.	1.9	16
3237	Molecular dynamics simulations reveal the effect of mutations in the RING domains of BRCA1-BARD1 complex and its relevance to the prognosis of breast cancer. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 12734-12752.	2.0	1

#	ARTICLE	IF	CITATIONS
3238	Unsupervised cross-domain translation via deep learning and adversarial attention neural networks and application to music-inspired protein designs. <i>Patterns</i> , 2023, 4, 100692.	3.1	6
3240	Preferential recovery and separation of rhodium in the concentrated hydrochloric acid using thin-layer oil membrane extraction based on laminar flow. <i>Chemical Engineering Research and Design</i> , 2023, 192, 69-81.	2.7	1
3241	Regulatory Mechanism of Opposite Charges on Chiral Self-Assembly of Cellulose Nanocrystals. <i>Molecules</i> , 2023, 28, 1857.	1.7	0
3242	Molecular dynamics simulations reveal the importance of amyloid-beta oligomer β^2 -sheet edge conformations in membrane permeabilization. <i>Journal of Biological Chemistry</i> , 2023, 299, 103034.	1.6	6
3243	Quantitative structural assessments of potential meprin β^2 inhibitors by non-linear QSAR approaches and validation by binding mode of interaction analysis. <i>New Journal of Chemistry</i> , 2023, 47, 7051-7069.	1.4	11
3244	Detailed analysis of distorted retinal and its interaction with surrounding residues in the K intermediate of bacteriorhodopsin. <i>Communications Biology</i> , 2023, 6, .	2.0	2
3245	Four flavonoids from propolis ameliorate free fatty acids-induced non-alcoholic steatohepatitis in HepG2 cells: Involvement of enhanced AMPK activation, mTOR-NF- κ Bp65 interaction, and PTEN expression. <i>Journal of Functional Foods</i> , 2023, 102, 105460.	1.6	1
3246	Concentration-Dependent Inhibition of Mesophilic PETases on Poly(ethylene terephthalate) Can Be Eliminated by Enzyme Engineering. <i>ChemSusChem</i> , 2023, 16, .	3.6	9
3247	Discovery of 4-(1,2,4-Oxadiazol-5-yl)azepan-2-one Derivatives as a New Class of Cannabinoid Type 2 Receptor Agonists for the Treatment of Inflammatory Pain. <i>Journal of Medicinal Chemistry</i> , 2023, 66, 3460-3483.	2.9	1
3248	In silico prediction of potential inhibitors for SARS-CoV-2 Omicron variant using molecular docking and dynamics simulation-based drug repurposing. <i>Journal of Molecular Modeling</i> , 2023, 29, .	0.8	2
3249	To the Understanding of Catalysis by D-Amino Acid Transaminases: A Case Study of the Enzyme from <i>Aminobacterium colombiense</i> . <i>Molecules</i> , 2023, 28, 2109.	1.7	2
3250	Revealing the Key Packing Features Determining the Stability of Peptide Bilayer Membrane. <i>ACS Applied Bio Materials</i> , 2024, 7, 564-578.	2.3	2
3251	A computational study on the biotransformation of alkenylbenzenes by a selection of CYPs: Reflections on their possible bioactivation. <i>Toxicology</i> , 2023, 488, 153471.	2.0	2
3252	Insights into the Substrate Uptake Mechanism of <i>Mycobacterium Tuberculosis</i> Ribose 5-Phosphate Isomerase and Perspectives on Drug Development. <i>Biophysica</i> , 2023, 3, 139-157.	0.6	0
3253	Molecular Dynamics Assessment of Mechanical Properties of the Thin Filaments in Cardiac Muscle. <i>International Journal of Molecular Sciences</i> , 2023, 24, 4792.	1.8	1
3254	Effect of Fc core fucosylation and light chain isotype on IgG1 flexibility. <i>Communications Biology</i> , 2023, 6, .	2.0	0
3256	Microscopic Understanding of the Conformational Stability of the Aggregated Nonamyloid β^2 Components of β^2 -Synuclein. <i>Journal of Chemical Information and Modeling</i> , 2023, 63, 1542-1555.	2.5	0
3258	QM/MM Modeling of the Flavin Functionalization in the RutA Monooxygenase. <i>Molecules</i> , 2023, 28, 2405.	1.7	1

#	ARTICLE	IF	CITATIONS
3260	Activation mechanism of the human Smoothed receptor. <i>Biophysical Journal</i> , 2023, 122, 1400-1413.	0.2	6
3261	Allosteric communication in the gating mechanism for controlled protein degradation by the bacterial ClpP peptidase. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	4
3262	Stereo-complementary epoxidation of 4-vinyl-2,3-dihydrobenzofuran using mutants of SeStyA with enhanced stability and enantioselectivity. <i>Molecular Catalysis</i> , 2023, 540, 113055.	1.0	0
3264	Potential Energy Surfaces Sampled in Cremerâ€Pople Coordinates and Represented by Common Force Field Functionals for Small Cyclic Molecules. <i>Journal of Physical Chemistry A</i> , 2023, 127, 2646-2663.	1.1	0
3265	Biophysical and Integrative Characterization of Protein Intrinsic Disorder as a Prime Target for Drug Discovery. <i>Biomolecules</i> , 2023, 13, 530.	1.8	2
3266	Structures of ferroportin in complex with its specific inhibitor vamifeport. <i>ELife</i> , 0, 12, .	2.8	2
3267	Dynamic play between human N-Î±-acetyltransferase D and H4-mutant histones: Molecular dynamics study. <i>Current Protein and Peptide Science</i> , 2023, 24, .	0.7	0
3268	SARS-CoV-2 Protein S Fusion Peptide Is Capable of Wrapping Negatively-Charged Phospholipids. <i>Membranes</i> , 2023, 13, 344.	1.4	2
3269	Sappanin-type homoisoflavonoids from <i>Scilla nervosa</i> inhibits acetylcholinesterase enzyme: a combined in silico and in vitro approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 10957-10968.	2.0	1
3272	Investigation of Solid Formation Enthalpy and Molecular Mechanics Energies of Amino Acids via Force Field Approach. <i>Bitlis Eren Üniversitesi Fen Bilimleri Dergisi</i> , 2023, 12, 10-16.	0.1	0
3273	Characterization of RNA polymerase II trigger loop mutations using molecular dynamics simulations and machine learning. <i>PLoS Computational Biology</i> , 2023, 19, e1010999.	1.5	1
3274	Using Local Protein Model Quality Estimates to Guide a Molecular Dynamics-Based Refinement Strategy. <i>Methods in Molecular Biology</i> , 2023, , 119-140.	0.4	0
3275	Identification of nonhistone substrates of the lysine methyltransferase PRDM9. <i>Journal of Biological Chemistry</i> , 2023, 299, 104651.	1.6	3
3277	Statistical learning of protein elastic network from positional covariance matrix. <i>Computational and Structural Biotechnology Journal</i> , 2023, 21, 2524-2535.	1.9	1
3278	Understanding the Electronic Structure Basis for N ₂ Binding to FeMoco: A Systematic Quantum Mechanics/Molecular Mechanics Investigation. <i>Inorganic Chemistry</i> , 2023, 62, 5357-5375.	1.9	7
3279	Enhanced Interfacial H-Bond Networks Promote Glycanâ€Glycan Recognition and Interaction. <i>ACS Applied Materials & Interfaces</i> , 2023, 15, 17592-17600.	4.0	0
3280	Binding of Venezuelan Equine Encephalitis Virus Inhibitors to Importin-Î± Receptors Explored with All-Atom Replica Exchange Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2023, 127, 3175-3186.	1.2	1
3281	All-atom simulations of the trimeric spike protein of SARS-CoV-2 in aqueous medium: Nature of interactions, conformational stability and free energy diagrams for conformational transition of the protein. <i>Journal of Computational Chemistry</i> , 2023, 44, 1560-1577.	1.5	2

#	ARTICLE	IF	CITATIONS
3282	Integrating in Silico and In Vitro Studies to Screen Anti- <i>Staphylococcus aureus</i> Activity From Vietnamese <i>Ganoderma multiplicatum</i> and <i>Ganoderma sinense</i> . <i>Natural Product Communications</i> , 2023, 18, 1934578X2311672.	0.2	1
3284	Lysine Deacetylase Substrate Selectivity: Distinct Interaction Surfaces Drive Positive and Negative Selection for Residues Following Acetyllysine. <i>Biochemistry</i> , 2023, 62, 1464-1483.	1.2	2
3286	Labyrinthopeptin A2 disrupts raft domains. <i>Chemistry and Physics of Lipids</i> , 2023, 253, 105303.	1.5	1
3287	Targeting multidrug resistant <i>Staphylococcus aureus</i> with cationic chlorpromazine-peptide conjugates. <i>Chemistry - an Asian Journal</i> , 2023, 18, .	1.7	1
3288	Discovery of seven-membered ring berberine analogues as highly potent and specific hCES2A inhibitors. <i>Chemico-Biological Interactions</i> , 2023, 378, 110501.	1.7	3
3289	Machine Learning-Driven Multiscale Modeling: Bridging the Scales with a Next-Generation Simulation Infrastructure. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 2658-2675.	2.3	10
3290	O-GlcNAcylation promotes the cytosolic localization of the m6A reader YTHDF1 and colorectal cancer tumorigenesis. <i>Journal of Biological Chemistry</i> , 2023, 299, 104738.	1.6	7
3292	Dissecting the species-specific recognition of Neoseptin 3 by TLR4/MD2 via molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 0, , .	1.3	0
3294	Covalent Adduct Formation as a Strategy for Efficient CO ₂ Fixation in Crotonyl-CoA Carboxylases/Reductases. <i>ACS Catalysis</i> , 2023, 13, 6230-6241.	5.5	2
3295	De Novo Evolution of an Antibody-Mimicking Multivalent Aptamer via a DNA Framework. <i>Small Methods</i> , 2023, 7, .	4.6	1
3296	Computational design and molecular dynamics simulations suggest the mode of substrate binding in ceramide synthases. <i>Nature Communications</i> , 2023, 14, .	5.8	5
3297	Seipin concentrates distinct neutral lipids via interactions with their acyl chain carboxyl esters. <i>Journal of Cell Biology</i> , 2022, 221, .	2.3	10
3420	Molecular-dynamics simulations of macromolecular diffraction, part I: Preparation of protein crystal simulations. <i>Methods in Enzymology</i> , 2023, , .	0.4	1
3451	Application of Computational Techniques in Antibody Fc-Fused Molecule Design for Therapeutics. <i>Molecular Biotechnology</i> , 0, , .	1.3	0
3454	Intermolecular pair potentials and force fields. , 2024, , 51-116.		0
3499	Cosolute Interactions with Tryptophan Peptide. <i>Lecture Notes in Electrical Engineering</i> , 2023, , 559-570.	0.3	0
3677	Antibreast cancer oncological drugs. , 2024, , 209-243.		0
3680	Inhibition of gas hydrate growth. , 2024, , 423-477.		0

#	ARTICLE	IF	CITATIONS
3683	Simulating chemical reactions promoted by self-assembled peptides with catalytic properties. <i>Methods in Enzymology</i> , 2024, , .	0.4	0
3690	Characterization of Posttranslationally Modified PHF-1 Tau Peptides Using Gaussian Accelerated Molecular Dynamics Simulation. <i>Methods in Molecular Biology</i> , 2024, , 3-31.	0.4	0