Michael Feig

List of Publications by Year
in descending order

157 papers	21,988 citations	34105 52 h-index	10158 140 g-index
180 all docs	180 docs citations	180 times ranked	20414 citing authors

#	Article	IF	Citations
1	CHARMM36m: an improved force field for folded and intrinsically disordered proteins. Nature Methods, 2017, 14, 71-73.	19.0	3,959
2	Optimization of the Additive CHARMM All-Atom Protein Force Field Targeting Improved Sampling of the Backbone ï•, Ïˆ and Side-Chain Ï‡₁ and Ï‡₂ Dihedral Angles. Journal of Chemical Theory and Computation, 2012, 8, 3257-3273.	5.3	3,696
3	Extending the treatment of backbone energetics in protein force fields: Limitations of gas-phase quantum mechanics in reproducing protein conformational distributions in molecular dynamics simulations. Journal of Computational Chemistry, 2004, 25, 1400-1415.	3.3	3,145
4	Improved Treatment of the Protein Backbone in Empirical Force Fields. Journal of the American Chemical Society, 2004, 126, 698-699.	13.7	912
5	MMTSB Tool Set: enhanced sampling and multiscale modeling methods for applications in structural biology. Journal of Molecular Graphics and Modelling, 2004, 22, 377-395.	2.4	807
6	Performance comparison of generalized born and Poisson methods in the calculation of electrostatic solvation energies for protein structures. Journal of Computational Chemistry, 2004, 25, 265-284.	3.3	523
7	Recent advances in the development and application of implicit solvent models in biomolecule simulations. Current Opinion in Structural Biology, 2004, 14, 217-224.	5.7	521
8	New analytic approximation to the standard molecular volume definition and its application to generalized Born calculations. Journal of Computational Chemistry, 2003, 24, 1348-1356.	3.3	474
9	An Implicit Membrane Generalized Born Theory for the Study of Structure, Stability, and Interactions of Membrane Proteins. Biophysical Journal, 2003, 85, 2900-2918.	0.5	384
10	Solvation and Hydration of Proteins and Nucleic Acids:â€‰ A Theoretical View of Simulation and Experiment. Accounts of Chemical Research, 2002, 35, 376-384.	15.6	321
11	High order matched interface and boundary method for elliptic equations with discontinuous coefficients and singular sources. Journal of Computational Physics, 2006, 213, 1-30.	3.8	287
12	Biomolecular interactions modulate macromolecular structure and dynamics in atomistic model of a bacterial cytoplasm. ELife, 2016, 5, .	6.0	238
13	Sodium and Chlorine Ions as Part of the DNA Solvation Shell. Biophysical Journal, 1999, 77, 1769-1781.	0.5	211
14	Force Field Influence on the Observation of Ï€-Helical Protein Structures in Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2003, 107, 2831-2836.	2.6	204
15	Protein Crowding Affects Hydration Structure and Dynamics. Journal of the American Chemical Society, 2012, 134, 4842-4849.	13.7	189
16	A generalized Born formalism for heterogeneous dielectric environments: Application to the implicit modeling of biological membranes. Journal of Chemical Physics, 2005, 122, 124706.	3.0	177
17	A distinct type of glycerol-3-phosphate acyltransferase with sn -2 preference and phosphatase activity producing 2-monoacylglycerol. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 12040-12045.	7.1	169
18	GENESIS: a hybridâ€parallel and multiâ€scale molecular dynamics simulator with enhanced sampling algorithms for biomolecular and cellular simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 310-323.	14.6	166

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19	Diffusion of Solvent around Biomolecular Solutes: A Molecular Dynamics Simulation Study. Biophysical Journal, 1998, 75, 150-158.	0.5	149
20	Reduced Native State Stability in Crowded Cellular Environment Due to Proteinâ€“Protein Interactions. Journal of the American Chemical Society, 2013, 135, 3696-3701.	13.7	145
21	Implicit solvation based on generalized Born theory in different dielectric environments. Journal of Chemical Physics, 2004, 120, 903-911.	3.0	136
22	Crowding in Cellular Environments at an Atomistic Level from Computer Simulations. Journal of Physical Chemistry B, 2017, 121, 8009-8025.	2.6	136
23	Inclusion of Many-Body Effects in the Additive CHARMM Protein CMAP Potential Results in Enhanced Cooperativity of Î±-Helix and Î²-Hairpin Formation. Biophysical Journal, 2012, 103, 1045-1051.	0.5	130
24	Structural Equilibrium of DNA Represented with Different Force Fields. Biophysical Journal, 1998, 75, 134-149.	0.5	127
25	Variable Interactions between Protein Crowders and Biomolecular Solutes Are Important in Understanding Cellular Crowding. Journal of Physical Chemistry B, 2012, 116, 599-605.	2.6	127
26	Modeling high-resolution hydration patterns in correlation with DNA sequence and conformation 1 1Edited by B. Honig. Journal of Molecular Biology, 1999, 286, 1075-1095.	4.2	114
27	Molecular dynamics simulations of biological membranes and membrane proteins using enhanced conformational sampling algorithms. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1635-1651.	2.6	111
28	Evolution and Physics in Comparative Protein Structure Modeling. Accounts of Chemical Research, 2002, 35, 413-421.	15.6	103
29	Physicsâ€based protein structure refinement through multiple molecular dynamics trajectories and structure averaging. Proteins: Structure, Function and Bioinformatics, 2014, 82, 196-207.	2.6	100
30	Highly accurate biomolecular electrostatics in continuum dielectric environments. Journal of Computational Chemistry, 2008, 29, 87-97.	3.3	98
31	PRIMO/PRIMONA: A coarseâ€grained model for proteins and nucleic acids that preserves nearâ€atomistic accuracy. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1266-1281.	2.6	97
32	A molecular simulation picture of DNA hydration around A- and B-DNA. Biopolymers, 1998, 48, 199.	2.4	94
33	Slow-Down in Diffusion in Crowded Protein Solutions Correlates with Transient Cluster Formation. Journal of Physical Chemistry B, 2017, 121, 11072-11084.	2.6	93
34	PRIMO: A Transferable Coarse-Grained Force Field for Proteins. Journal of Chemical Theory and Computation, 2013, 9, 3769-3788.	5.3	87
35	Accurate reconstruction of all-atom protein representations from side-chain-based low-resolution models. Proteins: Structure, Function and Bioinformatics, 2000, 41, 86-97.	2.6	85
36	Protein Structure Refinement through Structure Selection and Averaging from Molecular Dynamics Ensembles. Journal of Chemical Theory and Computation, 2013, 9, 1294-1303.	5.3	85

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37	Multiâ€state modeling of Gâ€protein coupled receptors at experimental accuracy. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1873-1885.	2.6	84
38	Balancing an accurate representation of the molecular surface in generalized born formalisms with integrator stability in molecular dynamics simulations. Journal of Computational Chemistry, 2006, 27, 719-729.	3.3	80
39	Evaluating CASP4 predictions with physical energy functions. Proteins: Structure, Function and Bioinformatics, 2002, 49, 232-245.	2.6	78
40	Experiment vs Force Fields:Â DNA Conformation from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 1997, 101, 7361-7363.	2.6	75
41	Is Alanine Dipeptide a Good Model for Representing the Torsional Preferences of Protein Backbones?. Journal of Chemical Theory and Computation, 2008, 4, 1555-1564.	5.3	73
42	Complete atomistic model of a bacterial cytoplasm for integrating physics, biochemistry, and systems biology. Journal of Molecular Graphics and Modelling, 2015, 58, 1-9.	2.4	71
43	Accurate prediction of protonation state as a prerequisite for reliable MMâ€PB(GB)SA binding free energy calculations of HIVâ€1 protease inhibitors. Journal of Computational Chemistry, 2008, 29, 673-685.	3.3	70
44	Molecular Dynamics Simulations of Large Integral Membrane Proteins with an Implicit Membrane Model. Journal of Physical Chemistry B, 2006, 110, 548-556.	2.6	68
45	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.	7.1	68
46	Kinetics from Implicit Solvent Simulations of Biomolecules as a Function of Viscosity. Journal of Chemical Theory and Computation, 2007, 3, 1734-1748.	5.3	66
47	Implicit Solvent Simulations of DNA and DNAâ^'Protein Complexes:â€‰ Agreement with Explicit Solvent vs Experiment. Journal of Physical Chemistry B, 2006, 110, 17240-17251.	2.6	65
48	Local Protein Structure Refinement via Molecular Dynamics Simulations with locPREFMD. Journal of Chemical Information and Modeling, 2016, 56, 1304-1312.	5.4	65
49	Protein structure refinement via molecularâ€dynamics simulations: What works and what does not?. Proteins: Structure, Function and Bioinformatics, 2016, 84, 282-292.	2.6	60
50	RNA Polymerase II with Open and Closed Trigger Loops: Active Site Dynamics and Nucleic Acid Translocation. Biophysical Journal, 2010, 99, 2577-2586.	0.5	59
51	Dynamic Error Correction and Regulation of Downstream Bubble Opening by Human RNA Polymerase II. Molecular Cell, 2005, 18, 461-470.	9.7	58
52	Reaching new levels of realism in modeling biological macromolecules in cellular environments. Journal of Molecular Graphics and Modelling, 2013, 45, 144-156.	2.4	58
53	Computational protein structure refinement: almost there, yet still so far to go. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1307.	14.6	57
54	Extending the horizon: towards the efficient modeling of large biomolecular complexes in atomic detail. Theoretical Chemistry Accounts, 2006, 116, 194-205.	1.4	53

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55	Conformational Sampling of Peptides in the Presence of Protein Crowders from AA/CG-Multiscale Simulations. Journal of Physical Chemistry B, 2012, 116, 8610-8620.	2.6	53
56	Clustering and dynamics of crowded proteins near membranes and their influence on membrane bending. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 24562-24567.	7.1	52
57	Synthetic curcuminoids modulate the arachidonic acid metabolism of human platelet 12-lipoxygenase and reduce sprout formation of human endothelial cells. Molecular Cancer Therapeutics, 2006, 5, 1371-1382.	4.1	51
58	Conformational Sampling of Peptides in Cellular Environments. Biophysical Journal, 2008, 94, 747-759.	0.5	51
59	Aberrant activity of the DNA repair enzyme AlkB. Journal of Inorganic Biochemistry, 2004, 98, 856-861.	3.5	49
60	Highâ€accuracy protein structures by combining machineâ€learning with physicsâ€based refinement. Proteins: Structure, Function and Bioinformatics, 2020, 88, 637-642.	2.6	48
61	The Requirement for Mechanical Coupling Between Head and S2 Domains in Smooth Muscle Myosin ATPase Regulation and its Implications for Dimeric Motor Function. Journal of Molecular Biology, 2005, 345, 837-854.	4.2	47
62	Interionic Hydration Structures of NaCl in Aqueous Solution: A Combined Study of Quantum Mechanical Cluster Calculations and QM/EFP-MD Simulations. Journal of Physical Chemistry B, 2013, 117, 289-295.	2.6	47
63	Whole-Cell Models and Simulations in Molecular Detail. Annual Review of Cell and Developmental Biology, 2019, 35, 191-211.	9.4	47
64	Recent Advances in Transferable Coarse-Grained Modeling of Proteins. Advances in Protein Chemistry and Structural Biology, 2014, 96, 143-180.	2.3	46
65	DNA Bending Propensity in the Presence of Base Mismatches: Implications for DNA Repair. Journal of Physical Chemistry B, 2013, 117, 6194-6205.	2.6	45
66	Dynamic Heterogeneous Dielectric Generalized Born (DHDGB): An Implicit Membrane Model with a Dynamically Varying Bilayer Thickness. Journal of Chemical Theory and Computation, 2013, 9, 1709-1719.	5.3	43
67	Mutational and Computational Evidence That a Nickel-Transfer Tunnel in UreD Is Used for Activation of Klebsiella aerogenes Urease. Biochemistry, 2015, 54, 6392-6401.	2.5	41
68	Influence of protein crowder size on hydration structure and dynamics in macromolecular crowding. Chemical Physics Letters, 2017, 671, 63-70.	2.6	41
69	Prediction of protein loop conformations using multiscale modeling methods with physical energy scoring functions. Journal of Computational Chemistry, 2008, 29, 820-831.	3.3	40
70	Driven to nearâ€experimental accuracy by refinement via molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1263-1275.	2.6	40
71	New parallel computing algorithm of molecular dynamics for extremely huge scale biological systems. Journal of Computational Chemistry, 2021, 42, 231-241.	3.3	40
72	Sampling of nearâ€native protein conformations during protein structure refinement using a coarseâ€grained model, normal modes, and molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1345-1356.	2.6	39

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73	Effect of proteinâ€“protein interactions and solvent viscosity on the rotational diffusion of proteins in crowded environments. Physical Chemistry Chemical Physics, 2019, 21, 876-883.	2.8	39
74	Charge-driven condensation of RNA and proteins suggests broad role of phase separation in cytoplasmic environments. ELife, 2021, 10, .	6.0	38
75	High-resolution 3D models of Caulobacter crescentus chromosome reveal genome structural variability and organization. Nucleic Acids Research, 2018, 46, 3937-3952.	14.5	37
76	Energetic and Structural Details of the Trigger-Loop Closing Transition inÂRNA Polymerase II. Biophysical Journal, 2013, 105, 767-775.	0.5	36
77	Crystallographic water sites from a theoretical perspective. Structure, 1998, 6, 1351-1354.	3.3	35
78	What makes it difficult to refine protein models further via molecular dynamics simulations?. Proteins: Structure, Function and Bioinformatics, 2018, 86, 177-188.	2.6	35
79	Conformational coupling, bridge helix dynamics and active site dehydration in catalysis by RNA polymerase. Biochimica Et Biophysica Acta - Gene Regulatory Mechanisms, 2010, 1799, 575-587.	1.9	34
80	Modeling Crowded Environment in Molecular Simulations. Frontiers in Molecular Biosciences, 2019, 6, 86.	3.5	33
81	NTP-driven translocation and regulation of downstream template opening by multi-subunit RNA polymerases. Biochemistry and Cell Biology, 2005, 83, 486-496.	2.0	32
82	Conformations of an Adenine Bulge in a DNA Octamer and Its Influence on DNA Structure from Molecular Dynamics Simulations. Biophysical Journal, 2001, 81, 352-370.	0.5	31
83	Purification and Characterization of the FeII- and Î±-Ketoglutarate-Dependent Xanthine Hydroxylase from Aspergillus nidulans. Biochemistry, 2007, 46, 5293-5304.	2.5	31
84	Transferring the PRIMO Coarse-Grained Force Field to the Membrane Environment: Simulations of Membrane Proteins and Helixâ€“Helix Association. Journal of Chemical Theory and Computation, 2014, 10, 3459-3472.	5.3	31
85	PREFMD: a web server for protein structure refinement via molecular dynamics simulations. Bioinformatics, 2018, 34, 1063-1065.	4.1	31
86	Hybrid All-Atom/Coarse-Grained Simulations of Proteins by Direct Coupling of CHARMM and PRIMO Force Fields. Journal of Chemical Theory and Computation, 2017, 13, 5753-5765.	5.3	29
87	Conformational Sampling of Influenza Fusion Peptide in Membrane Bilayers as a Function of Termini and Protonation States. Journal of Physical Chemistry B, 2010, 114, 1407-1416.	2.6	28
88	Molecular Evidence for Functional Divergence and Decay of a Transcription Factor Derived from Whole-Genome Duplication in Arabidopsis thaliana. Plant Physiology, 2015, 168, 1717-1734.	4.8	28
89	Role of the essential light chain in the activation of smooth muscle myosin by regulatory light chain phosphorylation. Journal of Structural Biology, 2014, 185, 375-382.	2.8	27
90	DnaC traps DnaB as an open ring and remodels the domain that binds primase. Nucleic Acids Research, 2016, 44, 210-220.	14.5	27

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91	Base-Flipping Mechanism in Postmismatch Recognition by MutS. Biophysical Journal, 2011, 101, 2223-2231.	0.5	25
92	Conformational Preferences of DNA in Reduced Dielectric Environments. Journal of Physical Chemistry B, 2014, 118, 10874-10881.	2.6	25
93	Implicit Membrane Models for Membrane Protein Simulation. Methods in Molecular Biology, 2008, 443, 181-196.	0.9	25
94	Deciphering the Mismatch Recognition Cycle in MutS and MSH2-MSH6 Using Normal-Mode Analysis. Biophysical Journal, 2009, 96, 1707-1720.	0.5	24
95	Computational Simulation Strategies for Analysis of Multisubunit RNA Polymerases. Chemical Reviews, 2013, 113, 8546-8566.	47.7	24
96	Solvent Electronic Polarization Effects on Na⁺â€“Na⁺ and Cl^{â€“}â€“Cl^{â€“} Pair Associations in Aqueous Solution. Journal of Physical Chemistry B, 2013, 117, 9273-9279.	2.6	24
97	Five checkpoints maintaining the fidelity of transcription by RNA polymerases in structural and energetic details. Nucleic Acids Research, 2015, 43, 1133-1146.	14.5	24
98	Evidence That the Bacillus subtilis SpoIIGA Protein Is a Novel Type of Signal-transducing Aspartic Protease. Journal of Biological Chemistry, 2008, 283, 15287-15299.	3.4	23
99	Thermodynamics of Macromolecular Association in Heterogeneous Crowding Environments: Theoretical and Simulation Studies with a Simplified Model. Journal of Physical Chemistry B, 2016, 120, 11856-11865.	2.6	23
100	Crowded environment affects the activity and inhibition of the NS3/4A protease. Biochimie, 2020, 176, 169-180.	2.6	23
101	Conformational Change in MSH2-MSH6 upon Binding DNA Coupled to ATPase Activity. Biophysical Journal, 2009, 96, L63-L65.	0.5	22
102	RNA polymerase II flexibility during translocation from normal mode analysis. Proteins: Structure, Function and Bioinformatics, 2010, 78, 434-446.	2.6	22
103	Effect of Membrane Thickness on Conformational Sampling of Phospholamban from Computer Simulations. Biophysical Journal, 2010, 98, 805-814.	0.5	22
104	Reduced efficacy of a Src kinase inhibitor in crowded protein solution. Nature Communications, 2021, 12, 4099.	12.8	22
105	Large scale distributed data repository: design of a molecular dynamics trajectory database. Future Generation Computer Systems, 1999, 16, 101-110.	7.5	21
106	Density-Biased Sampling: A Robust Computational Method for Studying Pore Formation in Membranes. Journal of Chemical Theory and Computation, 2015, 11, 343-350.	5.3	21
107	A correlation-based method for the enhancement of scoring functions on funnel-shaped energy landscapes. Proteins: Structure, Function and Bioinformatics, 2006, 63, 155-164.	2.6	20
108	Differential Mismatch Recognition Specificities of Eukaryotic MutS Homologs, MutSÎ± and MutSÎ². Biophysical Journal, 2014, 106, 2483-2492.	0.5	20

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109	Challenges and opportunities in connecting simulations with experiments via molecular dynamics of cellular environments. Journal of Physics: Conference Series, 2018, 1036, 012010.	0.4	20
110	Prediction of Membrane Permeation of Drug Molecules by Combining an Implicit Membrane Model with Machine Learning. Journal of Chemical Information and Modeling, 2019, 59, 1147-1162.	5.4	20
111	Improved Sampling Strategies for Protein Model Refinement Based on Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2021, 17, 1931-1943.	5.3	19
112	Protein assembly and crowding simulations. Current Opinion in Structural Biology, 2022, 73, 102340.	5.7	18
113	Thermal Stability of Peptide Nucleic Acid Complexes. Journal of Physical Chemistry B, 2019, 123, 8168-8177.	2.6	17
114	Physicsâ€based protein structure refinement in the era of artificial intelligence. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1870-1887.	2.6	17
115	The Unorthodox SNAP50 Zinc Finger Domain Contributes to Cooperative Promoter Recognition by Human SNAPC. Journal of Biological Chemistry, 2006, 281, 31050-31060.	3.4	16
116	Interactions of Amino Acid Side-Chain Analogs within Membrane Environments. Journal of Physical Chemistry B, 2015, 119, 2877-2885.	2.6	16
117	Improved Force Fields for Peptide Nucleic Acids with Optimized Backbone Torsion Parameters. Journal of Chemical Theory and Computation, 2018, 14, 3603-3620.	5.3	16
118	Structural basis for the enantiospecificities ofR- andS-specific phenoxypropionate/Î±-ketoglutarate dioxygenases. Protein Science, 2006, 15, 1356-1368.	7.6	15
119	Interaction of intramembrane metalloprotease SpoIVFB with substrate Pro-ÏƒK. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E10677-E10686.	7.1	15
120	Structure refinement of membrane proteins via molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2018, 86, 738-750.	2.6	15
121	Role of conformational sampling of Ser16 and Thr17-phosphorylated phospholamban in interactions with SERCA. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 577-585.	2.6	14
122	Effect of flanking residues on the conformational sampling of the internal fusion peptide from Ebola virus. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1109-1117.	2.6	13
123	Kinetics of nucleotide entry into RNA polymerase active site provides mechanism for efficiency and fidelity. Biochimica Et Biophysica Acta - Gene Regulatory Mechanisms, 2017, 1860, 482-490.	1.9	12
124	Short disordered protein segment regulates cross-species transmission of a yeast prion. Nature Chemical Biology, 2020, 16, 756-765.	8.0	12
125	Intramolecular Diffusion in Î±-Synuclein: It Depends on How You Measure It. Biophysical Journal, 2018, 115, 1190-1199.	0.5	11
126	The phage L capsid decoration protein has a novel OB-fold and an unusual capsid binding strategy. ELife, 2019, 8, .	6.0	11

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127	Scoring confidence index: statistical evaluation of ligand binding mode predictions. Journal of Computer-Aided Molecular Design, 2009, 23, 289-299.	2.9	10
128	Molecular Mechanism by Which Palmitate Inhibits PKR Autophosphorylation. Biochemistry, 2011, 50, 1110-1119.	2.5	10
129	The Evolutionarily Conserved C-terminal Domains in the Mammalian Retinoblastoma Tumor Suppressor Family Serve as Dual Regulators of Protein Stability and Transcriptional Potency. Journal of Biological Chemistry, 2015, 290, 14462-14475.	3.4	10
130	Heterogeneous dielectric generalized <scp>B</scp>orn model with a van der <scp>W</scp>aals term provides improved association energetics of membraneâ€embedded transmembrane helices. Journal of Computational Chemistry, 2017, 38, 1308-1320.	3.3	10
131	Substrate specificity of SpoIIGA, a signal-transducing aspartic protease in Bacilli. Journal of Biochemistry, 2011, 149, 665-671.	1.7	9
132	Accelerating the Generalized Born with Molecular Volume and Solvent Accessible Surface Area Implicit Solvent Model Using Graphics Processing Units. Journal of Computational Chemistry, 2020, 41, 830-838.	3.3	9
133	The endoplasmic reticulum acetyltransferases ATase1/NAT8B and ATase2/NAT8 are differentially regulated to adjust engagement of the secretory pathway. Journal of Neurochemistry, 2020, 154, 404-423.	3.9	9
134	Molecular Dynamics Trajectory Compression with a Coarse-Grained Model. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2012, 9, 476-486.	3.0	8
135	Determination of Hydrophobic Lengths of Membrane Proteins with the HDGB Implicit Membrane Model. Journal of Chemical Information and Modeling, 2017, 57, 3032-3042.	5.4	8
136	Role of protein interactions in stabilizing canonical DNA features in simulations of DNA in crowded environments. BMC Biophysics, 2018, 11, 8.	4.4	7
137	Long-Range Signaling in MutS and MSH Homologs via Switching of Dynamic Communication Pathways. PLoS Computational Biology, 2016, 12, e1005159.	3.2	7
138	Discrimination of Native-like States of Membrane Proteins with Implicit Membrane-based Scoring Functions. Journal of Chemical Theory and Computation, 2017, 13, 3049-3059.	5.3	6
139	High-Performance Data Analysis on the Big Trajectory Data of Cellular Scale All-atom Molecular Dynamics Simulations. Journal of Physics: Conference Series, 2018, 1036, 012009.	0.4	6
140	Biosynthesis and trafficking of heme o and heme a: new structural insights and their implications for reaction mechanisms and prenylated heme transfer. Critical Reviews in Biochemistry and Molecular Biology, 2021, 56, 1-29.	5.2	5
141	Crowding affects structural dynamics and contributes to membrane association of the NS3/4A complex. Biophysical Journal, 2021, 120, 3795-3806.	0.5	5
142	Implicit Solvent Simulations of Biomolecules in Cellular Environments. Annual Reports in Computational Chemistry, 2008, , 107-121.	1.7	3
143	Conformational Sampling in Structure Prediction and Refinement with Atomistic and Coarse-Grained Models. , 2011, , 85-109.		3
144	Binding site multiplicity with fatty acid ligands: Implications for the regulation of PKR kinase autophosphorylation with palmitate. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2429-2442.	2.6	3

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145	Intrinsic Base-Pair Rearrangement in the Hairpin Ribozyme Directs RNA Conformational Sampling and Tertiary Interface Formation. Journal of Physical Chemistry B, 2016, 120, 10885-10898.	2.6	3
146	Accurate reconstruction of allâ€atom protein representations from sideâ€chainâ€based lowâ€resolution models. Proteins: Structure, Function and Bioinformatics, 2000, 41, 86-97.	2.6	3
147	Modeling Aqueous Solvent Effects through Local Properties of Water. , 0, , 93-126.		2
148	Molecular Simulation Methods. ACS Symposium Series, 2010, , 155-178.	0.5	2
149	Molecular Dynamics Simulations of Biomolecules in Cellular Environments. Molecular Science, 2017, 11, A0094.	0.2	2
150	Virtual Issue on Protein Crowding and Stability. Journal of Physical Chemistry B, 2021, 125, 10649-10651.	2.6	2
151	Implicit Solvent Force-Field Optimization. , 0, , 167-190.		1
152	Role of then+1 amino acid residue on the deamidation of asparagine in pentapeptides. Molecular Physics, 2015, 113, 3839-3848.	1.7	1
153	Modeling Protein Solubility in Implicit Solvent. , 0, , 191-207.		0
154	Molecular Dynamics Simulations of Biomolecules in a Polarizable Coarse-Grained Solvent. , 0, , 251-272.		0
155	Conformational sampling of S- and R-warfarin in polar solvents: Implications for stereoselective complex formation. Computational and Theoretical Chemistry, 2010, 949, 41-51.	1.5	0
156	On the Development of State-Specific Coarse-Grained Potentials of Water. , 0, , 233-250.		0
157	2P120 Conformational Sampling of Nucleic Acids in Cellular Environments(05A. Nucleic acid:) Tj ETQq1 1 0.784314 rgBT /Overlock 1	0.1	0