Michael Feig

List of Publications by Citations

165 papers	16,371 citations	49 h-index	127 g-index
180 ext. papers	19,487 ext. citations	5.7 avg, IF	6.99 L-index

#	Paper	IF	Citations
165	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, 1400-15	3.5	2792
164	Optimization of the additive CHARMM all-atom protein force field targeting improved sampling of the backbone □□ and side-chain (□1) and (□2) dihedral angles. *Journal of Chemical Theory and Computation*, **2012**, 8, 3257-3273	6.4	2511
163	CHARMM36m: an improved force field for folded and intrinsically disordered proteins. *Nature Methods*, **2017**, 14, 71-73	21.6	1819
162	Improved treatment of the protein backbone in empirical force fields. *Journal of the American Chemical Society*, **2004**, 126, 698-9	16.4	773
161	MMTSB Tool Set: enhanced sampling and multiscale modeling methods for applications in structural biology. *Journal of Molecular Graphics and Modelling*, **2004**, 22, 377-95	2.8	709
160	Recent advances in the development and application of implicit solvent models in biomolecule simulations. *Current Opinion in Structural Biology*, **2004**, 14, 217-24	8.1	485
159	Performance comparison of generalized born and Poisson methods in the calculation of electrostatic solvation energies for protein structures. *Journal of Computational Chemistry*, **2004**, 25, 265-84	3.5	465
158	New analytic approximation to the standard molecular volume definition and its application to generalized Born calculations. *Journal of Computational Chemistry*, **2003**, 24, 1348-56	3.5	435
157	An implicit membrane generalized born theory for the study of structure, stability, and interactions of membrane proteins. *Biophysical Journal*, **2003**, 85, 2900-18	2.9	346
156	Solvation and hydration of proteins and nucleic acids: a theoretical view of simulation and experiment. *Accounts of Chemical Research*, **2002**, 35, 376-84	24.3	302
155	High order matched interface and boundary method for elliptic equations with discontinuous coefficients and singular sources. *Journal of Computational Physics*, **2006**, 213, 1-30	4.1	238
154	Sodium and chlorine ions as part of the DNA solvation shell. *Biophysical Journal*, **1999**, 77, 1769-81	2.9	196
153	Force Field Influence on the Observation of □Helical Protein Structures in Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2003**, 107, 2831-2836	3.4	186
152	Biomolecular interactions modulate macromolecular structure and dynamics in atomistic model of a bacterial cytoplasm. *ELife*, **2016**, 5,	8.9	161
151	A generalized Born formalism for heterogeneous dielectric environments: application to the implicit modeling of biological membranes. *Journal of Chemical Physics*, **2005**, 122, 124706	3.9	154
150	Protein crowding affects hydration structure and dynamics. *Journal of the American Chemical Society*, **2012**, 134, 4842-9	16.4	146
149	Diffusion of solvent around biomolecular solutes: a molecular dynamics simulation study. *Biophysical Journal*, **1998**, 75, 150-8	2.9	143

148	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, 12040-5	11.5	137
147	Structural equilibrium of DNA represented with different force fields. *Biophysical Journal*, **1998**, 75, 134-49	2.9	125
146	Implicit solvation based on generalized Born theory in different dielectric environments. *Journal of Chemical Physics*, **2004**, 120, 903-11	3.9	124
145	Reduced native state stability in crowded cellular environment due to protein-protein interactions. *Journal of the American Chemical Society*, **2013**, 135, 3696-701	16.4	121
144	Modeling high-resolution hydration patterns in correlation with DNA sequence and conformation. *Journal of Molecular Biology*, **1999**, 286, 1075-95	6.5	108
143	GENESIS: a hybrid-parallel and multi-scale molecular dynamics simulator with enhanced sampling algorithms for biomolecular and cellular simulations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2015**, 5, 310-323	7.9	107
142	Inclusion of many-body effects in the additive CHARMM protein CMAP potential results in enhanced cooperativity of α-helix and β-hairpin formation. *Biophysical Journal*, **2012**, 103, 1045-51	2.9	105
141	Variable interactions between protein crowders and biomolecular solutes are important in understanding cellular crowding. *Journal of Physical Chemistry B*, **2012**, 116, 599-605	3.4	104
140	Evolution and physics in comparative protein structure modeling. *Accounts of Chemical Research*, **2002**, 35, 413-21	24.3	97
139	Crowding in Cellular Environments at an Atomistic Level from Computer Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 8009-8025	3.4	89
138	Highly accurate biomolecular electrostatics in continuum dielectric environments. *Journal of Computational Chemistry*, **2008**, 29, 87-97	3.5	89
137	Molecular dynamics simulations of biological membranes and membrane proteins using enhanced conformational sampling algorithms. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1635-51	3.8	88
136	Physics-based protein structure refinement through multiple molecular dynamics trajectories and structure averaging. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82 Suppl 2, 196-207	4.2	86
135	A molecular simulation picture of DNA hydration around A- and B-DNA. *Biopolymers*, **1998**, 48, 199-209	2.2	86
134	Accurate reconstruction of all-atom protein representations from side-chain-based low-resolution models. *Proteins: Structure, Function and Bioinformatics*, **2000**, 41, 86-97	4.2	80
133	PRIMO/PRIMONA: a coarse-grained model for proteins and nucleic acids that preserves near-atomistic accuracy. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1266-81	4.2	78
132	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, 719-29	3.5	78
131	Protein Structure Refinement through Structure Selection and Averaging from Molecular Dynamics Ensembles. *Journal of Chemical Theory and Computation*, **2013**, 9, 1294-1303	6.4	75

130	Evaluating CASP4 predictions with physical energy functions. *Proteins: Structure, Function and Bioinformatics*, **2002**, 49, 232-45	4.2	75
129	PRIMO: A Transferable Coarse-grained Force Field for Proteins. *Journal of Chemical Theory and Computation*, **2013**, 9, 3769-3788	6.4	71
128	Experiment vs Force Fields: DNA Conformation from Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **1997**, 101, 7361-7363	3.4	69
127	Molecular dynamics simulations of large integral membrane proteins with an implicit membrane model. *Journal of Physical Chemistry B*, **2006**, 110, 548-56	3.4	66
126	Is Alanine Dipeptide a Good Model for Representing the Torsional Preferences of Protein Backbones?. *Journal of Chemical Theory and Computation*, **2008**, 4, 1555-64	6.4	65
125	Slow-Down in Diffusion in Crowded Protein Solutions Correlates with Transient Cluster Formation. *Journal of Physical Chemistry B*, **2017**, 121, 11072-11084	3.4	62
124	Kinetics from Implicit Solvent Simulations of Biomolecules as a Function of Viscosity. *Journal of Chemical Theory and Computation*, **2007**, 3, 1734-48	6.4	59
123	Accurate prediction of protonation state as a prerequisite for reliable MM-PB(GB)SA binding free energy calculations of HIV-1 protease inhibitors. *Journal of Computational Chemistry*, **2008**, 29, 673-85	3.5	59
122	Implicit solvent simulations of DNA and DNA-protein complexes: agreement with explicit solvent vs experiment. *Journal of Physical Chemistry B*, **2006**, 110, 17240-51	3.4	57
121	Dynamic error correction and regulation of downstream bubble opening by human RNA polymerase II. *Molecular Cell*, **2005**, 18, 461-70	17.6	55
120	Protein structure refinement via molecular-dynamics simulations: What works and what does not?. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84 Suppl 1, 282-92	4.2	52
119	Computational protein structure refinement: Almost there, yet still so far to go. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1307	7.9	49
118	Reaching new levels of realism in modeling biological macromolecules in cellular environments. *Journal of Molecular Graphics and Modelling*, **2013**, 45, 144-56	2.8	49
117	Complete atomistic model of a bacterial cytoplasm for integrating physics, biochemistry, and systems biology. *Journal of Molecular Graphics and Modelling*, **2015**, 58, 1-9	2.8	49
116	RNA polymerase II with open and closed trigger loops: active site dynamics and nucleic acid translocation. *Biophysical Journal*, **2010**, 99, 2577-86	2.9	49
115	Conformational sampling of peptides in cellular environments. *Biophysical Journal*, **2008**, 94, 747-59	2.9	47
114	Extending the horizon: towards the efficient modeling of large biomolecular complexes in atomic detail. *Theoretical Chemistry Accounts*, **2006**, 116, 194-205	1.9	47
113	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, 1371-82	6.1	46

112	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, 837-54	6.5	45
111	Aberrant activity of the DNA repair enzyme AlkB. *Journal of Inorganic Biochemistry*, **2004**, 98, 856-61	4.2	45
110	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	11.5	43
109	Conformational sampling of peptides in the presence of protein crowders from AA/CG-multiscale simulations. *Journal of Physical Chemistry B*, **2012**, 116, 8610-20	3.4	42
108	Modeling of Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) Proteins by Machine Learning and Physics-Based Refinement **2020**,		42
107	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	6.4	40
106	Local Protein Structure Refinement via Molecular Dynamics Simulations with locPREFMD. *Journal of Chemical Information and Modeling*, **2016**, 56, 1304-12	6.1	39
105	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, 289-95	3.4	37
104	Prediction of protein loop conformations using multiscale modeling methods with physical energy scoring functions. *Journal of Computational Chemistry*, **2008**, 29, 820-31	3.5	37
103	Recent advances in transferable coarse-grained modeling of proteins. *Advances in Protein Chemistry and Structural Biology*, **2014**, 96, 143-80	5.3	33
102	Sampling of near-native protein conformations during protein structure refinement using a coarse-grained model, normal modes, and molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 1345-56	4.2	33
101	DNA bending propensity in the presence of base mismatches: implications for DNA repair. *Journal of Physical Chemistry B*, **2013**, 117, 6194-205	3.4	31
100	Crystallographic water sites from a theoretical perspective. *Structure*, **1998**, 6, 1351-4	5.2	31
99	NTP-driven translocation and regulation of downstream template opening by multi-subunit RNA polymerases. *Biochemistry and Cell Biology*, **2005**, 83, 486-96	3.6	31
98	Driven to near-experimental accuracy by refinement via molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 1263-1275	4.2	29
97	Conformations of an adenine bulge in a DNA octamer and its influence on DNA structure from molecular dynamics simulations. *Biophysical Journal*, **2001**, 81, 352-70	2.9	29
96	What makes it difficult to refine protein models further via molecular dynamics simulations?. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86 Suppl 1, 177-188	4.2	28
95	Influence of protein crowder size on hydration structure and dynamics in macromolecular crowding. *Chemical Physics Letters*, **2017**, 671, 63-70	2.5	27

94	Effect of protein-protein interactions and solvent viscosity on the rotational diffusion of proteins in crowded environments. *Physical Chemistry Chemical Physics*, **2019**, 21, 876-883	3.6	27
93	Transferring the PRIMO Coarse-Grained Force Field to the Membrane Environment: Simulations of Membrane Proteins and Helix-Helix Association. *Journal of Chemical Theory and Computation*, **2014**, 10, 3459-3472	6.4	26
92	Mutational and Computational Evidence That a Nickel-Transfer Tunnel in UreD Is Used for Activation of Klebsiella aerogenes Urease. *Biochemistry*, **2015**, 54, 6392-401	3.2	26
91	Conformational coupling, bridge helix dynamics and active site dehydration in catalysis by RNA polymerase. *Biochimica Et Biophysica Acta - Gene Regulatory Mechanisms*, **2010**, 1799, 575-87	6	26
90	Purification and characterization of the FeII- and alpha-ketoglutarate-dependent xanthine hydroxylase from Aspergillus nidulans. *Biochemistry*, **2007**, 46, 5293-304	3.2	26
89	Energetic and structural details of the trigger-loop closing transition in RNA polymerase II. *Biophysical Journal*, **2013**, 105, 767-75	2.9	25
88	Role of the essential light chain in the activation of smooth muscle myosin by regulatory light chain phosphorylation. *Journal of Structural Biology*, **2014**, 185, 375-82	3.4	25
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, 1407-16	3.4	25
86	Continuum Electrostatics Solvent Modeling with the Generalized Born Model127-165		25
85	Whole-Cell Models and Simulations in Molecular Detail. *Annual Review of Cell and Developmental Biology*, **2019**, 35, 191-211	12.6	24
84	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	6.4	23
83	Implicit membrane models for membrane protein simulation. *Methods in Molecular Biology*, **2008**, 443, 181-96	1.4	23
82	Deciphering the mismatch recognition cycle in MutS and MSH2-MSH6 using normal-mode analysis. *Biophysical Journal*, **2009**, 96, 1707-20	2.9	22
81	RNA polymerase II flexibility during translocation from normal mode analysis. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 434-46	4.2	22
80	DnaC traps DnaB as an open ring and remodels the domain that binds primase. *Nucleic Acids Research*, **2016**, 44, 210-20	20.1	21
79	Conformational preferences of DNA in reduced dielectric environments. *Journal of Physical Chemistry B*, **2014**, 118, 10874-81	3.4	21
78	Base-flipping mechanism in postmismatch recognition by MutS. *Biophysical Journal*, **2011**, 101, 2223-31	2.9	21
77	High-accuracy protein structures by combining machine-learning with physics-based refinement. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 637-642	4.2	21

76	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	11.5	21
75	Molecular Evidence for Functional Divergence and Decay of a Transcription Factor Derived from Whole-Genome Duplication in Arabidopsis thaliana. *Plant Physiology*, **2015**, 168, 1717-34	6.6	20
74	PREFMD: a web server for protein structure refinement via molecular dynamics simulations. *Bioinformatics*, **2018**, 34, 1063-1065	7.2	20
73	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	3.4	20
72	Effect of membrane thickness on conformational sampling of phospholamban from computer simulations. *Biophysical Journal*, **2010**, 98, 805-14	2.9	20
71	High-resolution 3D models of Caulobacter crescentus chromosome reveal genome structural variability and organization. *Nucleic Acids Research*, **2018**, 46, 3937-3952	20.1	19
70	Solvent electronic polarization effects on Na(+)-Na(+) and Cl(-)-Cl(-) pair associations in aqueous solution. *Journal of Physical Chemistry B*, **2013**, 117, 9273-9	3.4	19
69	Evidence that the Bacillus subtilis SpoIIGA protein is a novel type of signal-transducing aspartic protease. *Journal of Biological Chemistry*, **2008**, 283, 15287-99	5.4	19
68	A correlation-based method for the enhancement of scoring functions on funnel-shaped energy landscapes. *Proteins: Structure, Function and Bioinformatics*, **2006**, 63, 155-64	4.2	19
67	Five checkpoints maintaining the fidelity of transcription by RNA polymerases in structural and energetic details. *Nucleic Acids Research*, **2015**, 43, 1133-46	20.1	18
66	Differential mismatch recognition specificities of eukaryotic MutS homologs, MutS□and MutS□ *Biophysical Journal*, **2014**, 106, 2483-92	2.9	18
65	Conformational change in MSH2-MSH6 upon binding DNA coupled to ATPase activity. *Biophysical Journal*, **2009**, 96, L63-5	2.9	18
64	Modeling Crowded Environment in Molecular Simulations. *Frontiers in Molecular Biosciences*, **2019**, 6, 86	5.6	17
63	Density-biased sampling: a robust computational method for studying pore formation in membranes. *Journal of Chemical Theory and Computation*, **2015**, 11, 343-50	6.4	17
62	Computational simulation strategies for analysis of multisubunit RNA polymerases. *Chemical Reviews*, **2013**, 113, 8546-66	68.1	15
61	Interactions of amino acid side-chain analogs within membrane environments. *Journal of Physical Chemistry B*, **2015**, 119, 2877-85	3.4	15
60	Large scale distributed data repository: design of a molecular dynamics trajectory database. *Future Generation Computer Systems*, **1999**, 16, 101-110	7.5	14
59	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	6.1	14

58	Role of conformational sampling of Ser16 and Thr17-phosphorylated phospholamban in interactions with SERCA. *Biochimica Et Biophysica Acta - Biomembranes*, **2013**, 1828, 577-85	3.8	13
57	Developing Force Fields from the Microscopic Structure of Solutions: The KirkwoodBuff Approach55-76		13
56	The unorthodox SNAP50 zinc finger domain contributes to cooperative promoter recognition by human SNAPC. *Journal of Biological Chemistry*, **2006**, 281, 31050-60	5.4	13
55	Structure refinement of membrane proteins via molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86, 738-750	4.2	12
54	Structural basis for the enantiospecificities of R- and S-specific phenoxypropionate/alpha-ketoglutarate dioxygenases. *Protein Science*, **2006**, 15, 1356-68	6.3	12
53	Effect of flanking residues on the conformational sampling of the internal fusion peptide from Ebola virus. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 1109-17	4.2	11
52	Short disordered protein segment regulates cross-species transmission of a yeast prion. *Nature Chemical Biology*, **2020**, 16, 756-765	11.7	10
51	Interaction of intramembrane metalloprotease SpoIVFB with substrate Pro-*Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E10677-E10686	11.5	10
50	Scoring confidence index: statistical evaluation of ligand binding mode predictions. *Journal of Computer-Aided Molecular Design*, **2009**, 23, 289-99	4.2	10
49	Crowded environment affects the activity and inhibition of the NS3/4A protease. *Biochimie*, **2020**, 176, 169-180	4.6	10
48	Challenges and opportunities in connecting simulations with experiments via molecular dynamics of cellular environments. *Journal of Physics: Conference Series*, **2018**, 1036,	0.3	10
47	Improved Force Fields for Peptide Nucleic Acids with Optimized Backbone Torsion Parameters. *Journal of Chemical Theory and Computation*, **2018**, 14, 3603-3620	6.4	10
46	Thermal Stability of Peptide Nucleic Acid Complexes. *Journal of Physical Chemistry B*, **2019**, 123, 8168-8177	3.4	9
45	Molecular mechanism by which palmitate inhibits PKR autophosphorylation. *Biochemistry*, **2011**, 50, 1110-9	3.2	9
44	Heterogeneous dielectric generalized Born model with a van der Waals term provides improved association energetics of membrane-embedded transmembrane helices. *Journal of Computational Chemistry*, **2017**, 38, 1308-1320	3.5	8
43	New parallel computing algorithm of molecular dynamics for extremely huge scale biological systems. *Journal of Computational Chemistry*, **2021**, 42, 231-241	3.5	8
42	Improved Sampling Strategies for Protein Model Refinement Based on Molecular Dynamics Simulation. *Journal of Chemical Theory and Computation*, **2021**, 17, 1931-1943	6.4	8
41	Determination of Hydrophobic Lengths of Membrane Proteins with the HDGB Implicit Membrane Model. *Journal of Chemical Information and Modeling*, **2017**, 57, 3032-3042	6.1	7

40	Substrate specificity of SpoIIGA, a signal-transducing aspartic protease in Bacilli. *Journal of Biochemistry*, **2011**, 149, 665-71	3.1	7
39	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	3.5	7
38	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	6	6
37	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, 14462-75	5.4	6
36	Molecular dynamics trajectory compression with a coarse-grained model. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **2012**, 9, 476-86	3	6
35	Long-Range Signaling in MutS and MSH Homologs via Switching of Dynamic Communication Pathways. *PLoS Computational Biology*, **2016**, 12, e1005159	5	6
34	The phage L capsid decoration protein has a novel OB-fold and an unusual capsid binding strategy. *ELife*, **2019**, 8,	8.9	6
33	Discrimination of Native-like States of Membrane Proteins with Implicit Membrane-based Scoring Functions. *Journal of Chemical Theory and Computation*, **2017**, 13, 3049-3059	6.4	5
32	Physics-based protein structure refinement in the era of artificial intelligence. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 1870-1887	4.2	5
31	Reduced efficacy of a Src kinase inhibitor in crowded protein solution. *Nature Communications*, **2021**, 12, 4099	17.4	5
30	Intramolecular Diffusion in □Synuclein: It Depends on How You Measure It. *Biophysical Journal*, **2018**, 115, 1190-1199	2.9	5
29	Protein assembly and crowding simulations.. *Current Opinion in Structural Biology*, **2022**, 73, 102340	8.1	5
28	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	6	4
27	Fast Analytical Continuum Treatments of Solvation209-232		4
26	High-Performance Data Analysis on the Big Trajectory Data of Cellular Scale All-atom Molecular Dynamics Simulations. *Journal of Physics: Conference Series*, **2018**, 1036,	0.3	4
25	Charge-driven condensation of RNA and proteins suggests broad role of phase separation in cytoplasmic environments. *ELife*, **2021**, 10,	8.9	4
24	Binding site multiplicity with fatty acid ligands: implications for the regulation of PKR kinase autophosphorylation with palmitate. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 2429-42	4.2	3
23	Conformational Sampling in Structure Prediction and Refinement with Atomistic and Coarse-Grained Models **2011**, 85-109		3

22	Implicit Solvent Simulations of Biomolecules in Cellular Environments. *Annual Reports in Computational Chemistry*, **2008**, 107-121	1.8	3
21	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	3.4	3
20	Accurate reconstruction of all-atom protein representations from side-chain-based low-resolution models **2000**, 41, 86		3
19	Molecular Dynamics Simulations of Biomolecules in Cellular Environments. *Molecular Science*, **2017**, 11, A0094	0	2
18	Role of protein interactions in stabilizing canonical DNA features in simulations of DNA in crowded environments. *BMC Biophysics*, **2018**, 11, 8	0	2
17	Biosynthesis and trafficking of heme and heme : new structural insights and their implications for reaction mechanisms and prenylated heme transfer. *Critical Reviews in Biochemistry and Molecular Biology*, **2021**, 56, 640-668	8.7	2
16	Crowding affects structural dynamics and contributes to membrane association of the NS3/4A complex. *Biophysical Journal*, **2021**, 120, 3795-3806	2.9	2
15	Osmolyte Influence on Protein Stability: Perspectives of Theory and Experiment77-92		2
14	Role of the n+1 amino acid residue on the deamidation of asparagine in pentapeptides. *Molecular Physics*, **2015**, 113, 3839-3848	1.7	1
13	Modeling Aqueous Solvent Effects through Local Properties of Water93-126		1
12	Molecular Simulation Methods. *ACS Symposium Series*, **2010**, 155-178	0.4	1
11	Model-Free Solvent Modeling In Chemistry and Biochemistry Based on the Statistical Mechanics of Liquids31-54		1
10	Implicit Solvent Force-Field Optimization167-190		1
9	The phage L capsid decoration protein has a novel OB-fold and an unusual capsid binding strategy		1
8	High-Accuracy Protein Structures by Combining Machine-Learning with Physics-Based Refinement		1
7	2P120 Conformational Sampling of Nucleic Acids in Cellular Environments(05A. Nucleic acid: Structure & Property,Poster). *Seibutsu Butsuri*, **2013**, 53, S178	0	
6	On the Development of State-Specific Coarse-Grained Potentials of Water233-250		
5	Biomolecular Solvation in Theory and Experiment1-29		

List of Publications

4 Modeling Electrostatic Polarization in Biological Solvents273-308

3 Modeling Protein Solubility in Implicit Solvent191-207

2 Molecular Dynamics Simulations of Biomolecules in a Polarizable Coarse-Grained Solvent251-272

1 Conformational sampling of S- and R-warfarin in polar solvents: Implications for stereoselective complex formation. *Computational and Theoretical Chemistry*, **2010**, 949, 41-51