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List of Publications by Year
in descending order

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67 papers	1,185 citations	430874 18 h-index	454955 30 g-index
69 all docs	69 docs citations	69 times ranked	769 citing authors

#	Article	IF	Citations
1	A unified coarse-grained model of biological macromolecules based on mean-field multipoleâ€“multipole interactions. Journal of Molecular Modeling, 2014, 20, 2306.	1.8	123
2	Prediction of protein assemblies, the next frontier: The <scp>CASP14â€CAPRI</scp> experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1800-1823.	2.6	73
3	Lessons from application of the UNRES force field to predictions of structures of CASP10 targets. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 14936-14941.	7.1	62
4	UNRES server for physics-based coarse-grained simulations and prediction of protein structure, dynamics and thermodynamics. Nucleic Acids Research, 2018, 46, W304-W309.	14.5	56
5	WeFold: A coopetition for protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1850-1868.	2.6	48
6	A general method for the derivation of the functional forms of the effective energy terms in coarse-grained energy functions of polymers. I. Backbone potentials of coarse-grained polypeptide chains. Journal of Chemical Physics, 2017, 146, 124106.	3.0	48
7	Performance of protein-structure predictions with the physics-based UNRES force field in CASP11. Bioinformatics, 2016, 32, 3270-3278.	4.1	44
8	A general method for the derivation of the functional forms of the effective energy terms in coarse-grained energy functions of polymers. III. Determination of scale-consistent backbone-local and correlation potentials in the UNRES force field and force-field calibration and validation. Journal of Chemical Physics, 2019, 150, 155104.	3.0	42
9	Physics-Based Potentials for the Coupling between Backbone- and Side-Chain-Local Conformational States in the United Residue (UNRES) Force Field for Protein Simulations. Journal of Chemical Theory and Computation, 2015, 11, 817-831.	5.3	39
10	Determination of Effective Potentials for the Stretching of C^{Î±}Â·Â·Â·C^{Î±} Virtual Bonds in Polypeptide Chains for Coarse-Grained Simulations of Proteins from ab Initio Energy Surfaces of N-Methylacetamide and N-Acetylpyrrolidine. Journal of Chemical Theory and Computation, 2012, 8, 1334-1343.	5.3	31
11	Improvement of the Treatment of Loop Structures in the UNRES Force Field by Inclusion of Coupling between Backbone- and Side-Chain-Local Conformational States. Journal of Chemical Theory and Computation, 2013, 9, 4620-4632.	5.3	30
12	Molecular dynamics insights into proteinâ€glycosaminoglycan systems from microsecondâ€scale simulations. Biopolymers, 2019, 110, e23252.	2.4	30
13	Theory and Practice of Coarse-Grained Molecular Dynamics of Biologically Important Systems. Biomolecules, 2021, 11, 1347.	4.0	29
14	Assessment of chemicalâ€crosslinkâ€assisted protein structure modeling in CASP13. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1283-1297.	2.6	27
15	Folding and Self-Assembly of a Small Protein Complex. Journal of Chemical Theory and Computation, 2012, 8, 3416-3422.	5.3	23
16	Extension of UNRES Force Field to Treat Polypeptide Chains with <scp>d</scp>-Amino Acid Residues. Journal of Chemical Theory and Computation, 2012, 8, 4746-4757.	5.3	20
17	Scale-consistent approach to the derivation of coarse-grained force fields for simulating structure, dynamics, and thermodynamics of biopolymers. Progress in Molecular Biology and Translational Science, 2020, 170, 73-122.	1.7	20
18	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. Scientific Reports, 2018, 8, 9939.	3.3	19

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19	Evaluation of the scale-consistent UNRES force field in template-free prediction of protein structures in the CASP13 experiment. Journal of Molecular Graphics and Modelling, 2019, 92, 154-166.	2.4	19
20	Introduction of periodic boundary conditions into <scp>UNRES</scp> force field. Journal of Computational Chemistry, 2015, 36, 940-946.	3.3	18
21	Physics-Based Potentials for Coarse-Grained Modeling of Proteinâ€“DNA Interactions. Journal of Chemical Theory and Computation, 2015, 11, 1792-1808.	5.3	18
22	Introduction of steered molecular dynamics into UNRES coarseâ€grained simulations package. Journal of Computational Chemistry, 2017, 38, 553-562.	3.3	18
23	Modeling protein structures with the coarse-grained UNRES force field in the CASP14 experiment. Journal of Molecular Graphics and Modelling, 2021, 108, 108008.	2.4	17
24	Peierls-Nabarro barrier and protein loop propagation. Physical Review E, 2014, 90, 062717.	2.1	16
25	Revised Backbone-Virtual-Bond-Angle Potentials to Treat the <scp>l</scp>- and <scp>d</scp>-Amino Acid Residues in the Coarse-Grained United Residue (UNRES) Force Field. Journal of Chemical Theory and Computation, 2014, 10, 2194-2203.	5.3	16
26	A new protein nucleicâ€acid coarseâ€grained force field based on the UNRES and NARESâ€2P force fields. Journal of Computational Chemistry, 2018, 39, 2360-2370.	3.3	16
27	What Makes Telomeres Unique?. Journal of Physical Chemistry B, 2017, 121, 2207-2219.	2.6	15
28	Dynamics of Disulfide-Bond Disruption and Formation in the Thermal Unfolding of Ribonuclease A. Journal of Chemical Theory and Computation, 2017, 13, 5721-5730.	5.3	15
29	Disulfide-Linked Peptides for Blocking BTLA/HVEM Binding. International Journal of Molecular Sciences, 2020, 21, 636.	4.1	15
30	Modeling the Structure, Dynamics, and Transformations of Proteins with the UNRES Force Field. Methods in Molecular Biology, 2022, 2376, 399-416.	0.9	14
31	Extension of the UNRES Coarse-Grained Force Field to Membrane Proteins in the Lipid Bilayer. Journal of Physical Chemistry B, 2019, 123, 7829-7839.	2.6	13
32	On the need to introduce environmental characteristics in ab initio protein structure prediction using a coarse-grained UNRES force field. Journal of Molecular Graphics and Modelling, 2022, 114, 108166.	2.4	12
33	Thermal unfolding of myoglobin in the Landau-Ginzburg-Wilson approach. Physical Review E, 2016, 94, 062405.	2.1	11
34	The molecular mechanism of structural changes in the antimicrobial peptide CM15 upon complex formation with drug molecule suramin: a computational analysis. Physical Chemistry Chemical Physics, 2019, 21, 10644-10659.	2.8	11
35	Improved Consensus-Fragment Selection in Template-Assisted Prediction of Protein Structures with the UNRES Force Field in CASP13. Journal of Chemical Information and Modeling, 2020, 60, 1844-1864.	5.4	11
36	Investigation of Phosphorylation-Induced Folding of an Intrinsically Disordered Protein by Coarse-Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 3203-3220.	5.3	11

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37	Mitochondrial potassium channels: A novel calcitriol target. Cellular and Molecular Biology Letters, 2022, 27, 3.	7.0	11
38	Inhibitory activity of doubleâ€sequence analogues of trypsin inhibitor SFTIâ€1 from sunflower seeds: an example of peptide splicing. FEBS Journal, 2010, 277, 2351-2359.	4.7	10
39	Molecular dynamics of protein A and a WW domain with a united-residue model including hydrodynamic interaction. Journal of Chemical Physics, 2016, 144, 184110.	3.0	10
40	Introduction of Phosphorylated Residues into the UNRES Coarse-Grained Model: Toward Modeling of Signaling Processes. Journal of Physical Chemistry B, 2019, 123, 5721-5729.	2.6	10
41	Fluorescent analogs of trypsin inhibitor SFTIâ€1 isolated from sunflower seedsâ€”synthesis and applications. Biopolymers, 2014, 102, 124-135.	2.4	9
42	Studies of conformational changes of an arginine-binding protein from Thermotoga maritima in the presence and absence of ligand via molecular dynamics simulations with the coarse-grained UNRES force field. Journal of Molecular Modeling, 2015, 21, 64.	1.8	9
43	Bloch spin waves and emergent structure in protein folding with HIV envelope glycoprotein as an example. Physical Review E, 2016, 93, 032409.	2.1	9
44	Fragments of gD Protein as Inhibitors of BTLA/HVEM Complex Formation - Design, Synthesis, and Cellular Studies. International Journal of Molecular Sciences, 2020, 21, 8876.	4.1	9
45	Role of the sulfur to Î±-carbon thioether bridges in thurincin H. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2868-2879.	3.5	8
46	Prediction of DNA and RNA structure with the NARES-2P force field and conformational space annealing. Physical Chemistry Chemical Physics, 2018, 20, 19656-19663.	2.8	8
47	Targeting the HVEM protein using a fragment of glycoprotein D to inhibit formation of the BTLA/HVEM complex. Bioorganic Chemistry, 2022, 122, 105748.	4.1	7
48	Extension of coarse-grained UNRES force field to treat carbon nanotubes. Journal of Molecular Modeling, 2018, 24, 121.	1.8	6
49	A structural model of the immune checkpoint CD160-HVEM complex derived from HDX-mass spectrometry and molecular modeling. Oncotarget, 2019, 10, 536-550.	1.8	6
50	Shielding effect in protein folding. Journal of Molecular Graphics and Modelling, 2018, 79, 118-132.	2.4	5
51	Truncation of Huia versabilis Bowman-Birk inhibitor increases its selectivity, matriptase-1 inhibitory activity and proteolytic stability. Biochimie, 2020, 171-172, 178-186.	2.6	5
52	Extension of the Unres Package for Physics-Based Coarse-Grained Simulations of Proteins and Protein Complexes to Very Large Systems. Biophysical Journal, 2021, 120, 83a-84a.	0.5	5
53	Folding and self-assembly of a small heterotetramer. Journal of Chemical Physics, 2014, 140, 105103.	3.0	4
54	Prediction of CD28-CD86 protein complex structure using different level of resolution approach. Journal of Molecular Graphics and Modelling, 2021, 103, 107802.	2.4	4

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55	Computational Studies of the Mechanical Stability for Single-Strand Break DNA. Journal of Physical Chemistry B, 2018, 122, 8166-8173.	2.6	3
56	Structural Characterization of Covalently Stabilized Human Cystatin C Oligomers. International Journal of Molecular Sciences, 2020, 21, 5860.	4.1	3
57	Theoretical investigation of the structural insights of the interactions of Î³-Fe2O3 nanoparticle with (EMIM TFSI) ionic liquid. Journal of Molecular Liquids, 2021, 340, 117198.	4.9	3
58	Coarse-grained modeling of the calcium, sodium, magnesium and potassium cations interacting with proteins. Journal of Molecular Modeling, 2022, 28, .	1.8	3
59	Solitons and protein folding: An In Silico experiment. AIP Conference Proceedings, 2015, , .	0.4	2
60	Theoretical Investigation of the Coronavirus SARS-CoV-2 (COVID-19) Infection Mechanism and Selectivity. Molecules, 2022, 27, 2080.	3.8	2
61	Microscopic Physics-Based Models of Proteins and Nucleic Acids. , 2017, , 67-120.		1
62	High Performance Computing with Coarse Grained Model of Biological Macromolecules. Supercomputing Frontiers and Innovations, 2018, 5, .	0.4	1
63	Physics-Based Coarse-Grained Modeling in Bio- and Nanochemistry. , 2022, , 31-69.		1
64	Origin of the Architecture of Biological Macromolecules - A Mean-Field Perspective. Biophysical Journal, 2014, 106, 256a.	0.5	0
65	A Novel Method for Force-Field Calibration Based on Maximum-Likelihood Approach and Thermal Unfolding Data. Biophysical Journal, 2015, 108, 158a.	0.5	0
66	A Rigorous Approach to Derive Analytical Expressions in Coarse-Grained Force Fields. Biophysical Journal, 2016, 110, 329a.	0.5	0
67	Formation of Secondary and Supersecondary Structure of Proteins as a Result of Coupling Between Local and Backbone-Electrostatic Interactions: A View Through Cluster-Cumulant Scope. Methods in Molecular Biology, 2019, 1958, 133-146.	0.9	0