PaweÅ, Krupa

List of Publications by Year
in descending order

42	918	471061 17	476904 29
papers	citations	h-index	g-index

45	45	45	749
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Physics-Based Coarse-Grained Modeling in Bio- and Nanochemistry. , 2022, , 31-69.		1
2	Modeling the Structure, Dynamics, and Transformations of Proteins with the UNRES Force Field. Methods in Molecular Biology, 2022, 2376, 399-416.	0.4	14
3	Bis-coumarin homodimersâ€"potential inhibitors of amyloid aggregation of globular and intrinsically disordered proteins. Biophysical Journal, 2022, 121, 189a.	0.2	0
4	Computational Models for the Study of Protein Aggregation. Methods in Molecular Biology, 2022, 2340, 51-78.	0.4	2
5	Amyloid Î² Dodecamer Disrupts the Neuronal Membrane More Strongly than the Mature Fibril: Understanding the Role of Oligomers in Neurotoxicity. Journal of Physical Chemistry B, 2022, 126, 3659-3672.	1.2	9
6	UNRES-Dockâ€"proteinâ€"protein and peptideâ€"protein docking by coarse-grained replica-exchange MD simulations. Bioinformatics, 2021, 37, 1613-1615.	1.8	14
7	Prediction of CD28-CD86 protein complex structure using different level of resolution approach. Journal of Molecular Graphics and Modelling, 2021, 103, 107802.	1.3	4
8	Plant isoquinoline alkaloids as potential neurodrugs: A comparative study of the effects of benzo[c]phenanthridine and berberine-based compounds on Î²-amyloid aggregation. Chemico-Biological Interactions, 2021, 334, 109300.	1.7	27
9	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.	0.2	5
10	Modeling protein structures with the coarse-grained UNRES force field in the CASP14 experiment. Journal of Molecular Graphics and Modelling, 2021, 108, 108008.	1.3	17
11	Computational Model to Unravel the Function of Amyloid-Î² Peptides in Contact with a Phospholipid Membrane. Journal of Physical Chemistry B, 2020, 124, 3300-3314.	1.2	7
12	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.	2.5	11
13	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.	0.9	20
14	Properties of monomeric AÎ²42 probed by different sampling methods and force fields: Role of energy components. Journal of Chemical Physics, 2019, 151, .	1.2	26
15	Structure and Physicochemical Properties of the AÎ²42 Tetramer: Multiscale Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2019, 123, 7253-7269.	1.2	25
16	Blind prediction of homoâ€•and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	1.5	99
17	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.	1.3	19
18	Prediction of protein structure with the coarseâ€grained UNRES force field assisted by small Xâ€ray scattering data and knowledgeâ€based information. Proteins: Structure, Function and Bioinformatics, 2018, 86, 228-239.	1.5	26

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19	Reoptimized UNRES Potential for Protein Model Quality Assessment. Genes, 2018, 9, 601.	1.0	2
20	Use of the UNRES force field in template-assisted prediction of protein structures and the refinement of server models: Test with CASP12 targets. Journal of Molecular Graphics and Modelling, 2018, 83, 92-99.	1.3	19
21	Computational Studies of the Mechanical Stability for Single-Strand Break DNA. Journal of Physical Chemistry B, 2018, 122, 8166-8173.	1.2	3
22	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. Scientific Reports, 2018, 8, 9939.	1.6	19
23	Use of Coarse-Grained and All-Atom Molecular Dynamics to Study Hsp70 and Hsp40 Chaperone Action. Frontiers in Structural Biology, 2018, , 23-46.	0.3	0
24	What Makes Telomeres Unique?. Journal of Physical Chemistry B, 2017, 121, 2207-2219.	1.2	15
25	Ergodicity and model quality in templateâ€restrained canonical and temperature/Hamiltonian replica exchange coarseâ€grained molecular dynamics simulations of proteins. Journal of Computational Chemistry, 2017, 38, 2730-2746.	1.5	8
26	Dynamics of Disulfide-Bond Disruption and Formation in the Thermal Unfolding of Ribonuclease A. Journal of Chemical Theory and Computation, 2017, 13, 5721-5730.	2.3	15
27	Maximum Likelihood Calibration of the UNRES Force Field for Simulation of Protein Structure and Dynamics. Journal of Chemical Information and Modeling, 2017, 57, 2364-2377.	2.5	38
28	Inhibitors or toxins? Large library target-specific screening of fullerene-based nanoparticles for drug design purpose. Nanoscale, 2017, 9, 10263-10276.	2.8	29
29	Role of the sulfur to Î±-carbon thioether bridges in thurincin H. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2868-2879.	2.0	8
30	Microscopic Physics-Based Models of Proteins and Nucleic Acids. , 2017, , 67-120.		1
31	Performance of protein-structure predictions with the physics-based UNRES force field in CASP11. Bioinformatics, 2016, 32, 3270-3278.	1.8	44
32	Use of Restraints from Consensus Fragments of Multiple Server Models To Enhance Protein-Structure Prediction Capability of the UNRES Force Field. Journal of Chemical Information and Modeling, 2016, 56, 2263-2279.	2.5	15
33	Molecular modeling of the binding modes of the iron-sulfur protein to the Jac1 co-chaperone from S accharomyces cerevisiae by all-atom and coarse-grained approaches. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1414-1426.	1.5	32
34	Prediction of Protein Structure by Template-Based Modeling Combined with the UNRES Force Field. Journal of Chemical Information and Modeling, 2015, 55, 1271-1281.	2.5	16
35	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.	2.3	39
36	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.	0.8	9

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37	Preventing fibril formation of a protein by selective mutation. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 13549-13554.	3.3	17
38	Origin of the Architecture of Biological Macromolecules - A Mean-Field Perspective. Biophysical Journal, 2014, 106, 256a.	0.2	0
39	WeFold: A coopetition for protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1850-1868.	1.5	48
40	A unified coarse-grained model of biological macromolecules based on mean-field multipoleâ€“multipole interactions. Journal of Molecular Modeling, 2014, 20, 2306.	0.8	123
41	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.	2.3	30
42	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.	3.3	62