Adam K Sieradzan

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	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.	0.9	14
3	Mitochondrial potassium channels: A novel calcitriol target. Cellular and Molecular Biology Letters, 2022, 27, 3.	7.0	11
4	Theoretical Investigation of the Coronavirus SARS-CoV-2 (COVID-19) Infection Mechanism and Selectivity. Molecules, 2022, 27, 2080.	3.8	2
5	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
6	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
7	Coarse-grained modeling of the calcium, sodium, magnesium and potassium cations interacting with proteins. Journal of Molecular Modeling, 2022, 28, .	1.8	3
8	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
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.	0.5	5
10	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
11	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
12	Theory and Practice of Coarse-Grained Molecular Dynamics of Biologically Important Systems. Biomolecules, 2021, 11, 1347.	4.0	29
13	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
14	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
15	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
16	Structural Characterization of Covalently Stabilized Human Cystatin C Oligomers. International Journal of Molecular Sciences, 2020, 21, 5860.	4.1	3
17	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
18	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

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19	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
20	Disulfide-Linked Peptides for Blocking BTLA/HVEM Binding. International Journal of Molecular Sciences, 2020, 21, 636.	4.1	15
21	Assessment of chemicalâ€crosslinkâ€assisted protein structure modeling in CASP13. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1283-1297.	2.6	27
22	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
23	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
24	Molecular dynamics insights into proteinâ€glycosaminoglycan systems from microsecondâ€scale simulations. Biopolymers, 2019, 110, e23252.	2.4	30
25	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
26	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
27	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
28	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
29	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
30	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
31	Extension of coarse-grained UNRES force field to treat carbon nanotubes. Journal of Molecular Modeling, 2018, 24, 121.	1.8	6
32	Shielding effect in protein folding. Journal of Molecular Graphics and Modelling, 2018, 79, 118-132.	2.4	5
33	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
34	Computational Studies of the Mechanical Stability for Single-Strand Break DNA. Journal of Physical Chemistry B, 2018, 122, 8166-8173.	2.6	3
35	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
36	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

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37	High Performance Computing with Coarse Grained Model of Biological Macromolecules. Supercomputing Frontiers and Innovations, 2018, 5, .	0.4	1
38	Introduction of steered molecular dynamics into UNRES coarseâ€grained simulations package. Journal of Computational Chemistry, 2017, 38, 553-562.	3.3	18
39	What Makes Telomeres Unique?. Journal of Physical Chemistry B, 2017, 121, 2207-2219.	2.6	15
40	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
41	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
42	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
43	Microscopic Physics-Based Models of Proteins and Nucleic Acids. , 2017, , 67-120.		1
44	Performance of protein-structure predictions with the physics-based UNRES force field in CASP11. Bioinformatics, 2016, 32, 3270-3278.	4.1	44
45	Thermal unfolding of myoglobin in the Landau-Ginzburg-Wilson approach. Physical Review E, 2016, 94, 062405.	2.1	11
46	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
47	A Rigorous Approach to Derive Analytical Expressions in Coarse-Grained Force Fields. Biophysical Journal, 2016, 110, 329a.	0.5	0
48	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
49	A Novel Method for Force-Field Calibration Based on Maximum-Likelihood Approach and Thermal Unfolding Data. Biophysical Journal, 2015, 108, 158a.	0.5	0
50	Solitons and protein folding: An In Silico experiment. AIP Conference Proceedings, 2015, , .	0.4	2
51	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
52	Introduction of periodic boundary conditions into <scp>UNRES</scp> force field. Journal of Computational Chemistry, 2015, 36, 940-946.	3.3	18
53	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
54	Physics-Based Potentials for Coarse-Grained Modeling of Proteinâ€“DNA Interactions. Journal of Chemical Theory and Computation, 2015, 11, 1792-1808.	5.3	18

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55	Peierls-Nabarro barrier and protein loop propagation. Physical Review E, 2014, 90, 062717.	2.1	16
56	Folding and self-assembly of a small heterotetramer. Journal of Chemical Physics, 2014, 140, 105103.	3.0	4
57	Fluorescent analogs of trypsin inhibitor SFTIâ€1 isolated from sunflower seedsâ€"synthesis and applications. Biopolymers, 2014, 102, 124-135.	2.4	9
58	Origin of the Architecture of Biological Macromolecules - A Mean-Field Perspective. Biophysical Journal, 2014, 106, 256a.	0.5	0
59	WeFold: A coopetition for protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1850-1868.	2.6	48
60	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
61	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
62	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
63	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
64	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
65	Folding and Self-Assembly of a Small Protein Complex. Journal of Chemical Theory and Computation, 2012, 8, 3416-3422.	5.3	23
66	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
67	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