Adam Liwo

List of Publications by Year
in descending order

242	7,973	53794 45	74163 75
papers	citations	h-index	g-index

248	248	248	4921
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Principal Component Analysis for Protein Folding Dynamics. Journal of Molecular Biology, 2009, 385, 312-329.	4.2	331
2	Protein-Folding Dynamics: Overview of Molecular Simulation Techniques. Annual Review of Physical Chemistry, 2007, 58, 57-83.	10.8	329
3	Ab initio simulations of protein-folding pathways by molecular dynamics with the united-residue model of polypeptide chains. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 2362-2367.	7.1	256
4	Cumulant-based expressions for the multibody terms for the correlation between local and electrostatic interactions in the united-residue force field. Journal of Chemical Physics, 2001, 115, 2323-2347.	3.0	236
5	Modification and Optimization of the United-Residue (UNRES) Potential Energy Function for Canonical Simulations. I. Temperature Dependence of the Effective Energy Function and Tests of the Optimization Method with Single Training Proteins. Journal of Physical Chemistry B, 2007, 111, 260-285.	2.6	184
6	Computational techniques for efficient conformational sampling of proteins. Current Opinion in Structural Biology, 2008, 18, 134-139.	5.7	170
7	Polyproline II conformation is one of many local conformational states and is not an overall conformation of unfolded peptides and proteins. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 1744-1749.	7.1	156
8	Molecular Dynamics with the United-Residue Model of Polypeptide Chains. II. Langevin and Berendsen-Bath Dynamics and Tests on Model Î±-Helical Systems. Journal of Physical Chemistry B, 2005, 109, 13798-13810.	2.6	144
9	Relation between Free Energy Landscapes of Proteins and Dynamics. Journal of Chemical Theory and Computation, 2010, 6, 583-595.	5.3	132
10	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
11	A method for optimizing potential-energy functions by a hierarchical design of the potential-energy landscape: Application to the UNRES force field. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 1937-1942.	7.1	122
12	Molecular Dynamics with the United-Residue Model of Polypeptide Chains. I. Lagrange Equations of Motion and Tests of Numerical Stability in the Microcanonical Mode. Journal of Physical Chemistry B, 2005, 109, 13785-13797.	2.6	114
13	Parametrization of Backboneâ€'Electrostatic and Multibody Contributions to the UNRES Force Field for Protein-Structure Prediction from Ab Initio Energy Surfaces of Model Systemsâ€. Journal of Physical Chemistry B, 2004, 108, 9421-9438.	2.6	113
14	A general method for the determination of the stoichiometry of unknown species in multicomponent systems from physicochemical measurements. Computers & Chemistry, 1987, 11, 195-210.	1.2	105
15	Blind prediction of homoâ€•and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	2.6	99
16	Calculation of protein conformation by global optimization of a potential energy function. Proteins: Structure, Function and Bioinformatics, 1999, 37, 204-208.	2.6	96
17	CAS MCSCF/CAS MCQDPT2 Study of the Mechanism of Singlet Oxygen Addition to 1,3-Butadiene and Benzene. Journal of the American Chemical Society, 2000, 122, 8112-8119.	13.7	95
18	Application of Multiplexed Replica Exchange Molecular Dynamics to the UNRES Force Field: Tests with Î± and Î±+Î² Proteins. Journal of Chemical Theory and Computation, 2009, 5, 627-640.	5.3	93

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19	Investigation of Protein Folding by Coarse-Grained Molecular Dynamics with the UNRES Force Field. Journal of Physical Chemistry A, 2010, 114, 4471-4485.	2.5	91
20	Molecular simulation study of cooperativity in hydrophobic association. Protein Science, 2000, 9, 1235-1245.	7.6	90
21	Mechanism of Fiber Assembly: Treatment of AÎ² Peptide Aggregation with a Coarse-Grained United-Residue Force Field. Journal of Molecular Biology, 2010, 404, 537-552.	4.2	87
22	Coupling Between Folding and Ionization Equilibria: Effects of pH on the Conformational Preferences of Polypeptides. Journal of Molecular Biology, 1996, 264, 770-783.	4.2	85
23	Potential of Mean Force of Association of Large Hydrophobic Particles: Toward the Nanoscale Limit. Journal of Physical Chemistry B, 2010, 114, 993-1003.	2.6	79
24	Mean-Field Interactions between Nucleic-Acid-Base Dipoles can Drive the Formation of a Double Helix. Physical Review Letters, 2013, 110, 098101.	7.8	74
25	Optimization of the UNRES Force Field by Hierarchical Design of the Potential-Energy Landscape. 3. Use of Many Proteins in Optimization. Journal of Physical Chemistry B, 2004, 108, 16950-16959.	2.6	73
26	Coarse-grained force field: general folding theory. Physical Chemistry Chemical Physics, 2011, 13, 16890.	2.8	73
27	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
28	Optimization of the UNRES Force Field by Hierarchical Design of the Potential-Energy Landscape. 2. Off-Lattice Tests of the Method with Single Proteins. Journal of Physical Chemistry B, 2004, 108, 16934-16949.	2.6	68
29	Kinetic Studies of Folding of the B-domain of Staphylococcal Protein A with Molecular Dynamics and a United-residue (UNRES) Model of Polypeptide Chains. Journal of Molecular Biology, 2006, 355, 536-547.	4.2	66
30	Î²-hairpin-forming peptides; models of early stages of protein folding. Biophysical Chemistry, 2010, 151, 1-9.	2.8	65
31	Development of Physics-Based Energy Functions that Predict Medium-Resolution Structures for Proteins of the Î±, Î², and Î±/Î² Structural Classes. Journal of Physical Chemistry B, 2001, 105, 7299-7311.	2.6	64
32	Exploring the parameter space of the coarseâ€grained UNRES force field by random search: Selecting a transferable mediumâ€resolution force field. Journal of Computational Chemistry, 2009, 30, 2127-2135.	3.3	64
33	Potential of Mean Force of Hydrophobic Association:â€‰ Dependence on Solute Size. Journal of Physical Chemistry B, 2007, 111, 10765-10774.	2.6	63
34	Simulation of the Opening and Closing of Hsp70 Chaperones by Coarse-Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2012, 8, 1750-1764.	5.3	63
35	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
36	Exploration of the conformational space of oxytocin and arginine-vasopressin using the electrostatically driven Monte Carlo and molecular dynamics methods. , 1998, 38, 157-175.		61

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37	Determination of the Potentials of Mean Force for Rotation about CÎ±â"CÎ±Virtual Bonds in Polypeptides from the ab Initio Energy Surfaces of Terminally Blocked Glycine, Alanine, and Prolineâ€. Journal of Physical Chemistry A, 2003, 107, 8035-8046.	2.5	60
38	Electrochemical and UV-spectrophotometric study of oxygen and superoxide anion radical interaction with anthraquinone derivatives and their radical anions. Electrochimica Acta, 2000, 45, 3581-3587.	5.2	56
39	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
40	A Study of the Î±-Helical Intermediate Preceding the Aggregation of the Amino-Terminal Fragment of the Î² Amyloid Peptide (AÎ²_{1â€"28}). Journal of Physical Chemistry B, 2011, 115, 12978-12983.	2.6	53
41	Further Evidence for the Absence of Polyproline II Stretch in the XAO Peptide. Biophysical Journal, 2007, 92, 2904-2917.	0.5	51
42	New developments of the electrostatically driven monte carlo method: Test on the membrane-bound portion of melittin. , 1998, 46, 117-126.		49
43	Molecular dynamics study of a gelsolin-derived peptide binding to a lipid bilayer containing phosphatidylinositol 4,5-bisphosphate. Biopolymers, 2003, 71, 49-70.	2.4	49
44	Conformational Dynamics of the Trp-Cage Miniprotein at Its Folding Temperature. Journal of Physical Chemistry B, 2012, 116, 6898-6907.	2.6	49
45	How Adequate are One- and Two-Dimensional Free Energy Landscapes for Protein Folding Dynamics?. Physical Review Letters, 2009, 102, 238102.	7.8	48
46	WeFold: A coopetition for protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1850-1868.	2.6	48
47	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
48	Diffusion Equation and Distance Scaling Methods of Global Optimization:Â Applications to Crystal Structure Prediction. Journal of Physical Chemistry A, 1998, 102, 2904-2918.	2.5	46
49	Molecular Dynamics with the United-Residue Force Field:Â Ab Initio Folding Simulations of Multichain Proteins. Journal of Physical Chemistry B, 2007, 111, 293-309.	2.6	46
50	Implementation of Molecular Dynamics and Its Extensions with the Coarse-Grained UNRES Force Field on Massively Parallel Systems: Toward Millisecond-Scale Simulations of Protein Structure, Dynamics, and Thermodynamics. Journal of Chemical Theory and Computation, 2010, 6, 890-909.	5.3	46
51	Energy-based reconstruction of a protein backbone from its ?-carbon trace by a Monte-Carlo method. Journal of Computational Chemistry, 2002, 23, 715-723.	3.3	45
52	Performance of protein-structure predictions with the physics-based UNRES force field in CASP11. Bioinformatics, 2016, 32, 3270-3278.	4.1	44
53	An Improved Functional Form for the Temperature Scaling Factors of the Components of the Mesoscopic UNRES Force Field for Simulations of Protein Structure and Dynamics. Journal of Physical Chemistry B, 2009, 113, 8738-8744.	2.6	42
54	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

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55	Electrochemical study of oxygen interaction with lapachol and its radical anions. Bioelectrochemistry, 2003, 59, 85-87.	4.6	40
56	Photophysical Properties of Tyrosine and Its Simple Derivatives Studied by Time-Resolved Fluorescence Spectroscopy, Global Analysis, and Theoretical Calculations. Journal of Physical Chemistry B, 2004, 108, 3879-3889.	2.6	40
57	Implementation of a symplectic multiple-time-step molecular dynamics algorithm, based on the united-residue mesoscopic potential energy function. Journal of Chemical Physics, 2006, 125, 204107.	3.0	40
58	PDZ Binding to the BAR Domain of PICK1 is Elucidated by Coarse-grained Molecular Dynamics. Journal of Molecular Biology, 2011, 405, 298-314.	4.2	40
59	DNA Duplex Formation with a Coarse-Grained Model. Journal of Chemical Theory and Computation, 2014, 10, 5020-5035.	5.3	39
60	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
61	Insights into the structure and dynamics of lysyl oxidase propeptide, a flexible protein with numerous partners. Scientific Reports, 2018, 8, 11768.	3.3	39
62	Efficient parallel algorithms in global optimization of potential energy functions for peptides, proteins, and crystals. Computer Physics Communications, 2000, 128, 399-411.	7.5	38
63	Implementations of NosÃ©â€“Hoover and NosÃ©â€“PoincarÃ© thermostats in mesoscopic dynamic simulations with the united-residue model of a polypeptide chain. Journal of Chemical Physics, 2008, 128, 245103.	3.0	38
64	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.	5.4	38
65	An Efficient Deformation-Based Global Optimization Method (Self-Consistent Basin-to-Deformed-Basin) Tj ETQq1 1 0.784314 rgBT /O 1999, 103, 9370-9377.	2.5	37
66	Topology of Type II REases revisited; structural classes and the common conserved core. Nucleic Acids Research, 2007, 35, 2227-2237.	14.5	37
67	Hierarchical energy-based approach to protein-structure prediction: Blind-test evaluation with CASP3 targets. International Journal of Quantum Chemistry, 2000, 77, 90-117.	2.0	36
68	Can cooperativity in hydrophobic association be reproduced correctly by implicit solvation models?. International Journal of Quantum Chemistry, 2002, 88, 41-55.	2.0	36
69	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force for the Interaction of Amino Acid Side Chains in Water. IV. Pairs of Different Hydrophobic Side Chains. Journal of Physical Chemistry B, 2008, 112, 11385-11395.	2.6	36
70	Determination of sideâ€chainâ€rotamer and sideâ€chain and backbone virtualâ€bondâ€stretching potentials of mean force from AM1 energy surfaces of terminallyâ€blocked aminoâ€acid residues, for coarseâ€grained simulations of protein structure and folding. II. Results, comparison with statistical potentials, and implementation in the UNRES force field. Journal of Computational Chemistry, 2010, 31, 1154-1167.	3.3	36
71	Folding kinetics of WW domains with the united residue force field for bridging microscopic motions and experimental measurements. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 18243-18248.	7.1	36
72	Comparison of the low energy conformations of an oncogenic and a non-oncogenic p21 protein, neither of which binds GTP or GDP. The Protein Journal, 1994, 13, 237-251.	1.1	35

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73	Improved conformational space annealing method to treat Î²-structure with the UNRES force-field and to enhance scalability of parallel implementation. Polymer, 2004, 45, 677-686.	3.8	34
74	A Maximum-Likelihood Approach to Force-Field Calibration. Journal of Chemical Information and Modeling, 2015, 55, 2050-2070.	5.4	34
75	Addition of side chains to a known backbone with defined side-chain centroids. Biophysical Chemistry, 2002, 100, 261-280.	2.8	33
76	Molecular Simulation Study of the Potentials of Mean Force for the Interactions between Models of Like-Charged and between Charged and Nonpolar Amino Acid Side Chains in Water. Journal of Physical Chemistry B, 2003, 107, 13496-13504.	2.6	33
77	Prediction of the structures of proteins with the UNRES force field, including dynamic formation and breaking of disulfide bonds. Protein Engineering, Design and Selection, 2004, 17, 29-36.	2.1	33
78	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force for the Interaction of Amino Acid Side Chains in Water. 3. Calculation and Parameterization of the Potentials of Mean Force of Pairs of Identical Hydrophobic Side Chains. Journal of Physical Chemistry B, 2007, 111, 2925-2931.	2.6	33
79	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.	2.6	32
80	Evidence, from Simulations, of a Single State with Residual Native Structure at the Thermal Denaturation Midpoint of a Small Globular Protein. Journal of the American Chemical Society, 2010, 132, 9444-9452.	13.7	31
81	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
82	Molecular simulation study of cooperativity in hydrophobic association: clusters of four hydrophobic particles. Biophysical Chemistry, 2003, 105, 339-359.	2.8	30
83	Optimization of the UNRES Force Field by Hierarchical Design of the Potential-Energy Landscape. 1. Tests of the Approach Using Simple Lattice Protein Models. Journal of Physical Chemistry B, 2004, 108, 16918-16933.	2.6	30
84	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force of the Interaction of Amino-Acid Side Chains in Water. VI. Oppositely Charged Side Chains. Journal of Physical Chemistry B, 2011, 115, 6130-6137.	2.6	30
85	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
86	Surmounting the Multiple-Minima Problem in Protein Folding. Journal of Global Optimization, 1999, 15, 235-260.	1.8	29
87	Molecular Origin of Anticooperativity in Hydrophobic Association. Journal of Physical Chemistry B, 2005, 109, 8108-8119.	2.6	29
88	Theory and Practice of Coarse-Grained Molecular Dynamics of Biologically Important Systems. Biomolecules, 2021, 11, 1347.	4.0	29
89	Theoretical and electrochemical study of the mechanism of anthraquinone-mediated one-electron reduction of oxygen: the involvement of adducts of dioxygen species to anthraquinones. Journal of the Chemical Society Perkin Transactions II, 1997, , 229-236.	0.9	28
90	Coarseâ€grained model of nucleic acid bases. Journal of Computational Chemistry, 2010, 31, 1644-1655.	3.3	28

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91	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force of the Interaction of Amino-Acid Side Chains in Water. V. Like-Charged Side Chains. Journal of Physical Chemistry B, 2011, 115, 6119-6129.	2.6	28
92	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force for the Interaction of Amino Acid Side Chains in Water. 2. Tests with Simple Spherical Systems. Journal of Physical Chemistry B, 2007, 111, 2917-2924.	2.6	27
93	Assessment of chemicalâ€crosslinkâ€assisted protein structure modeling in CASP13. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1283-1297.	2.6	27
94	Ab Initio Study of Energetics of Protonation and Hydrogen Bonding of PyridineN-Oxide and Its Derivatives. Journal of Physical Chemistry A, 1999, 103, 11104-11108.	2.5	26
95	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.	2.6	26
96	Prediction of protein structure using a knowledge-based off-lattice united-residue force field and global optimization methods. Theoretical Chemistry Accounts, 1999, 101, 16-20.	1.4	25
97	Optimization of a Nucleic Acids united-RESidue 2-Point model (NARES-2P) with a maximum-likelihood approach. Journal of Chemical Physics, 2015, 143, 243111.	3.0	25
98	The role of the Val57 aminoâ€acid residue in the hinge loop of the human cystatin C. Conformational studies of the beta2â€1â€beta3 segments of wildâ€type human cystatin C and its mutants. Biopolymers, 2009, 91, 373-383.	2.4	24
99	Theoretical Studies on the Structure, Stability, Ability To Undergo Internal Transformations, and Tautomerization, as Well as Reactivity, of H2PPH2 and HPPH3 Molecules. Journal of the American Chemical Society, 1995, 117, 2638-2648.	13.7	23
100	Mechanism of formation of the Câ€terminal Î²â€hairpin of the B3 domain of the immunoglobulin binding protein G from Streptococcus. I. Importance of hydrophobic interactions in stabilization of Î²â€hairpin structure. Proteins: Structure, Function and Bioinformatics, 2009, 75, 931-953.	2.6	23
101	Folding and Self-Assembly of a Small Protein Complex. Journal of Chemical Theory and Computation, 2012, 8, 3416-3422.	5.3	23
102	Calculation of protein conformation by global optimization of a potential energy function. Proteins: Structure, Function and Bioinformatics, 1999, 37, 204-208.	2.6	23
103	Acidâ€“base and cationic homoconjugation equilibria of substituted pyridine N-oxides in acetone. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 3853-3856.	1.7	22
104	Evolution of physics-based methodology for exploring the conformational energy landscape of proteins. Journal of Computational Chemistry, 2002, 23, 28-34.	3.3	22
105	A united residue force-field for calcium-protein interactions. Protein Science, 2009, 13, 2725-2735.	7.6	22
106	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force for the Interaction of Amino Acid Side Chains in Water. 1. Approximate Expression for the Free Energy of Hydrophobic Association Based on a Gaussian-Overlap Model. Journal of Physical Chemistry B, 2007, 111, 2910-2916.	2.6	21
107	Electrochemical studies of isolapachol with emphasis on oxygen interaction with its radical anions. Journal of Electroanalytical Chemistry, 2004, 566, 25-29.	3.8	20
108	Towards temperature-dependent coarse-grained potentials of side-chain interactions for protein folding simulations. I: Molecular dynamics study of a pair of methane molecules in water at various temperatures. Protein Engineering, Design and Selection, 2009, 22, 547-552.	2.1	20

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109	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
110	Coexistence of Phases in a Protein Heterodimer. Journal of Chemical Physics, 2012, 137, 035101.	3.0	20
111	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
112	An Efficient Deformation-Based Global Optimization Method for Off-Lattice Polymer Chains:â€‰ Self-Consistent Basin-to-Deformed-Basin Mapping (SCBDBM). Application to United-Residue Polypeptide Chains. Journal of Physical Chemistry B, 1999, 103, 7353-7366.	2.6	19
113	Comment on â€œAnti-cooperativity in hydrophobic interactions: A simulation study of spatial dependence of three-body effects and beyondâ€•[J. Chem. Phys. 115, 1414 (2001)]. Journal of Chemical Physics, 2002, 116, 2665-2667.	3.0	19
114	Determination of virtual-bond-angle potentials of mean force for coarse-grained simulations of protein structure and folding fromab initioenergy surfaces of terminally-blocked glycine, alanine, and proline. Journal of Physics Condensed Matter, 2007, 19, 285203.	1.8	19
115	Determination of the pKa values of some biologically active and inactive hydroxyquinones. Journal of the Brazilian Chemical Society, 2008, 19, 175-183.	0.6	19
116	Accounting for a mirror-image conformation as a subtle effect in protein folding. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 8458-8463.	7.1	19
117	Simple Physics-Based Analytical Formulas for the Potentials of Mean Force of the Interaction of Amino Acid Side Chains in Water. VII. Chargedâ€“Hydrophobic/Polar and Polarâ€“Hydrophobic/Polar Side Chains. Journal of Physical Chemistry B, 2017, 121, 379-390.	2.6	19
118	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.	2.4	19
119	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
120	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
121	Introduction of a bounded penalty function in contactâ€assisted simulations of protein structures to omit false restraints. Journal of Computational Chemistry, 2019, 40, 2164-2178.	3.3	19
122	Comparison of two approaches to potential of mean force calculations of hydrophobic association: particle insertion and weighted histogram analysis methods. Molecular Physics, 2005, 103, 3153-3167.	1.7	18
123	Acidicâ€basic properties of three alanineâ€based peptides containing acidic and basic side chains: Comparison between theory and experiment. Biopolymers, 2008, 90, 724-732.	2.4	18
124	Influence of charge and size of terminal aminoâ€acid residues on local conformational states and shape of alanineâ€based peptides. Biopolymers, 2008, 90, 772-782.	2.4	18
125	Mechanism of formation of the Câ€terminal Î²â€hairpin of the B3 domain of the immunoglobulin binding protein G from Streptococcus. II. Interplay of local backbone conformational dynamics and longâ€range hydrophobic interactions in hairpin formation. Proteins: Structure, Function and Bioinformatics, 2009, 76, 637-654.	2.6	18
126	Local vs Global Motions in Protein Folding. Journal of Chemical Theory and Computation, 2013, 9, 2907-2921.	5.3	18

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127	Kinks, loops, and protein folding, with protein A as an example. Journal of Chemical Physics, 2014, 140, 025101.	3.0	18
128	Physics-Based Potentials for Coarse-Grained Modeling of Proteinâ€“DNA Interactions. Journal of Chemical Theory and Computation, 2015, 11, 1792-1808.	5.3	18
129	Relationship between the Electronic Structure and Acidic-Basic Properties of 4-Substituted Pyridine N-Oxides. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1989, 44, 1263-1270.	0.7	17
130	Absolute Stereochemistry of Soulattrolide and Its Analogues. Journal of Organic Chemistry, 1998, 63, 1233-1238.	3.2	17
131	Conformational solution studies of neuropeptide ? using CD and NMR spectroscopy. Journal of Peptide Science, 2002, 8, 211-226.	1.4	17
132	Mechanism of formation of the Câ€terminal Î²â€hairpin of the B3 domain of the immunoglobulinâ€binding protein G from Streptococcus. IV. Implication for the mechanism of folding of the parent protein. Biopolymers, 2010, 93, 469-480.	2.4	17
133	Effects of Mutation, Truncation, and Temperature on the Folding Kinetics of a WW Domain. Journal of Molecular Biology, 2012, 420, 350-365.	4.2	17
134	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
135	Assessment of Two Theoretical Methods to Estimate Potentiometric Titration Curves of Peptides:Â Comparison with Experiment. Journal of Physical Chemistry B, 2006, 110, 4451-4458.	2.6	16
136	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
137	Prediction of Protein Structure by Template-Based Modeling Combined with the UNRES Force Field. Journal of Chemical Information and Modeling, 2015, 55, 1271-1281.	5.4	16
138	In situ data analytics and indexing of protein trajectories. Journal of Computational Chemistry, 2017, 38, 1419-1430.	3.3	16
139	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
140	Theoretical Calculations of Heteroconjugation Equilibrium Constants in Systems Modeling Acidâ^'Base Interactions in Side Chains of Biomolecules Using the Potential of Mean Force. Journal of Physical Chemistry B, 2004, 108, 12222-12230.	2.6	15
141	Determination of sideâ€chainâ€rotamer and sideâ€chain and backbone virtualâ€bondâ€stretching potentials of mean force from AM1 energy surfaces of terminallyâ€blocked aminoâ€acid residues, for coarseâ€grained simulations of protein structure and folding. I. The method. Journal of Computational Chemistry, 2010, 31, 1143-1153.	3.3	15
142	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.	5.4	15
143	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
144	A study of cationic heteroconjugation equilibria of substituted pyridine N-oxides in acetonitrile. Analytica Chimica Acta, 1997, 338, 261-267.	5.4	14

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145	UNRES-Dockâ€"proteinâ€"protein and peptideâ€"protein docking by coarse-grained replica-exchange MD simulations. Bioinformatics, 2021, 37, 1613-1615.	4.1	14
146	Modeling the Structure, Dynamics, and Transformations of Proteins with the UNRES Force Field. Methods in Molecular Biology, 2022, 2376, 399-416.	0.9	14
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