Adam Liwo

List of Publications by Year in descending order

242 papers	7,973 citations	61687 45 h-index	84171 75 g-index
248 all docs	248 docs citations	248 times ranked	5619 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	Influence of Temperature and Salt Concentration on the Hydrophobic Interactions of Adamantane and Hexane. Journal of Physical Chemistry B, 2022, 126, 634-642.	1.2	2
4	Probing Protein Aggregation Using the Coarse-Grained UNRES Force Field. Methods in Molecular Biology, 2022, 2340, 79-104.	0.4	1
5	Theoretical Investigation of the Coronavirus SARS-CoV-2 (COVID-19) Infection Mechanism and Selectivity. Molecules, 2022, 27, 2080.	1.7	2
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	ESCASA : Analytical estimation of atomic coordinates from coarseâ€grained geometry for nuclearâ€magneticâ€resonance â€assisted protein structure modeling. I. Backbone and H Î² protons. Journal of Computational Chemistry, 2021, 42, 1579-1589.	1.5	4
8	Pseudopotentials for coarseâ€grained crossâ€linkâ€assisted modeling of protein structures. Journal of Computational Chemistry, 2021, 42, 2054-2067.	1.5	4
9	Prediction of protein assemblies, the next frontier: The <scp>CASP14â€CAPRI</scp> experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1800-1823.	1.5	73
10	Theory and Practice of Coarse-Grained Molecular Dynamics of Biologically Important Systems. Biomolecules, 2021, 11, 1347.	1.8	29
11	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
12	Extended disorder at the cell surface: The conformational landscape of the ectodomains of syndecans. Matrix Biology Plus, 2021, 12, 100081.	1.9	7
13	Recent Developments in Data-Assisted Modeling of Flexible Proteins. Frontiers in Molecular Biosciences, 2021, 8, 765562.	1.6	8
14	Unfolding the prospects of computational (bio)materials modeling. Journal of Chemical Physics, 2020, 153, 100901.	1.2	8
15	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
16	Hydrophobic hydration and pairwise hydrophobic interaction of Lennard-Jones and Mie particles in different water models. Physical Chemistry Chemical Physics, 2020, 22, 4758-4771.	1.3	4
17	Extension of the force-matching method to coarse-grained models with axially symmetric sites to produce transferable force fields: Application to the UNRES model of proteins. Journal of Chemical Physics, 2020, 152, 054902.	1.2	9
18	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

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19	Blind prediction of homoâ€•and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	1.5	99
20	Analysis of Procollagen C-Proteinase Enhancer-1/Glycosaminoglycan Binding Sites and of the Potential Role of Calcium Ions in the Interaction. International Journal of Molecular Sciences, 2019, 20, 5021.	1.8	11
21	Assessment of chemicalâ€crosslinkâ€assisted protein structure modeling in CASP13. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1283-1297.	1.5	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.	1.2	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.	1.3	19
24	Introduction of Phosphorylated Residues into the UNRES Coarse-Grained Model: Toward Modeling of Signaling Processes. Journal of Physical Chemistry B, 2019, 123, 5721-5729.	1.2	10
25	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.	1.3	11
26	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.	1.2	42
27	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.	1.5	19
28	Local and long range potentials for heparinâ€protein systems for coarseâ€grained simulations. Biopolymers, 2019, 110, e23269.	1.2	7
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.	0.4	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.	6.5	56
31	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
32	Reoptimized UNRES Potential for Protein Model Quality Assessment. Genes, 2018, 9, 601.	1.0	2
33	Impact of selected amino acids of HP0377 (Helicobacter pylori thiol oxidoreductase) on its functioning as a CcmG (cytochrome c maturation) protein and Dsb (disulfide bond) isomerase. PLoS ONE, 2018, 13, e0195358.	1.1	5
34	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.	1.5	16
35	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
36	Proteinâ€“Ligand Interaction Energy-Based Entropy Calculations: Fundamental Challenges For Flexible Systems. Journal of Physical Chemistry B, 2018, 122, 7821-7827.	1.2	11

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37	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
38	Prediction of DNA and RNA structure with the NARES-2P force field and conformational space annealing. Physical Chemistry Chemical Physics, 2018, 20, 19656-19663.	1.3	8
39	Insights into the structure and dynamics of lysyl oxidase propeptide, a flexible protein with numerous partners. Scientific Reports, 2018, 8, 11768.	1.6	39
40	In situ data analytics and indexing of protein trajectories. Journal of Computational Chemistry, 2017, 38, 1419-1430.	1.5	16
41	Chemoinformatics Methods for Studying Biomolecules. , 2017, , 2183-2199.		0
42	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.	1.2	48
43	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.	1.2	19
44	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
45	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
46	A general method for the derivation of the functional forms of the effective energy terms in coarse-grained energy functions of polymers. II. Backbone-local potentials of coarse-grained O1â†'4-bonded polyglucose chains. Journal of Chemical Physics, 2017, 147, 115101.	1.2	10
47	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
48	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
49	Microscopic Physics-Based Models of Proteins and Nucleic Acids. , 2017, , 67-120.		1
50	Performance of protein-structure predictions with the physics-based UNRES force field in CASP11. Bioinformatics, 2016, 32, 3270-3278.	1.8	44
51	Molecular dynamics of protein A and a WW domain with a united-residue model including hydrodynamic interaction. Journal of Chemical Physics, 2016, 144, 184110.	1.2	10
52	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
53	Chemoinformatics Methods for Studying Biomolecules. , 2016, , 1-17.		0
54	Optimization of a Nucleic Acids united-RESidue 2-Point model (NARES-2P) with a maximum-likelihood approach. Journal of Chemical Physics, 2015, 143, 243111.	1.2	25

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55	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
56	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
57	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
58	Theoretical Studies of Interactions between O-Phosphorylated and Standard Amino-Acid Side-Chain Models in Water. Journal of Physical Chemistry B, 2015, 119, 8526-8534.	1.2	4
59	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
60	Physics-Based Potentials for Coarse-Grained Modeling of Proteinâ€“DNA Interactions. Journal of Chemical Theory and Computation, 2015, 11, 1792-1808.	2.3	18
61	A Maximum-Likelihood Approach to Force-Field Calibration. Journal of Chemical Information and Modeling, 2015, 55, 2050-2070.	2.5	34
62	Common functionally important motions of the nucleotideâ€binding domain of H sp70. Proteins: Structure, Function and Bioinformatics, 2015, 83, 282-299.	1.5	4
63	Kinks, loops, and protein folding, with protein A as an example. Journal of Chemical Physics, 2014, 140, 025101.	1.2	18
64	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.	3.3	36
65	WeFold: A coopetition for protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1850-1868.	1.5	48
66	DNA Duplex Formation with a Coarse-Grained Model. Journal of Chemical Theory and Computation, 2014, 10, 5020-5035.	2.3	39
67	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
68	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.	2.3	16
69	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.	3.3	19
70	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
71	Coarse graining: a tool for large-scale simulations or more?. Physica Scripta, 2013, 87, 058502.	1.2	7
72	Mean-Field Interactions between Nucleic-Acid-Base Dipoles can Drive the Formation of a Double Helix. Physical Review Letters, 2013, 110, 098101.	2.9	74

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73	Local vs Global Motions in Protein Folding. Journal of Chemical Theory and Computation, 2013, 9, 2907-2921.	2.3	18
74	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
75	Multiple Î²â€sheet molecular dynamics of amyloid formation from two ABlâ€SH3 domain peptides. Biopolymers, 2012, 98, 557-566.	1.2	3
76	Influence of the Length of the Alanine Spacer on the Acidicâ€“Basic Properties of the Acâ€“Lysâ€“(Ala) n â€“Lysâ€“NH2 Peptides (nÂ=Â0, 1, 2, â€¦, 5). Journal of Solution Chemistry, 2012, 41, 1738-1746.	0.6	5
77	Simulation of the Opening and Closing of Hsp70 Chaperones by Coarse-Grained Molecular Dynamics. Journal of Chemical Theory and Computation, 2012, 8, 1750-1764.	2.3	63
78	Conformational Dynamics of the Trp-Cage Miniprotein at Its Folding Temperature. Journal of Physical Chemistry B, 2012, 116, 6898-6907.	1.2	49
79	Toward Temperature-Dependent Coarse-Grained Potentials of Side-Chain Interactions for Protein Folding Simulations. II. Molecular Dynamics Study of Pairs of Different Types of Interactions in Water at Various Temperatures. Journal of Physical Chemistry B, 2012, 116, 6844-6853.	1.2	7
80	Hidden Protein Folding Pathways in Free-Energy Landscapes Uncovered by Network Analysis. Journal of Chemical Theory and Computation, 2012, 8, 1176-1189.	2.3	13
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.	2.3	31
82	Folding and Self-Assembly of a Small Protein Complex. Journal of Chemical Theory and Computation, 2012, 8, 3416-3422.	2.3	23
83	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.	2.3	20
84	Effects of Mutation, Truncation, and Temperature on the Folding Kinetics of a WW Domain. Journal of Molecular Biology, 2012, 420, 350-365.	2.0	17
85	Coexistence of Phases in a Protein Heterodimer. Journal of Chemical Physics, 2012, 137, 035101.	1.2	20
86	Likeâ€charged residues at the ends of oligoalanine sequences might induce a chain reversal. Biopolymers, 2012, 97, 240-249.	1.2	8
87	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.	1.2	30
88	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.	1.2	53
89	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.	1.2	28
90	Coarse-grained force field: general folding theory. Physical Chemistry Chemical Physics, 2011, 13, 16890.	1.3	73

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91	PDZ Binding to the BAR Domain of PICK1 is Elucidated by Coarse-grained Molecular Dynamics. Journal of Molecular Biology, 2011, 405, 298-314.	2.0	40
92	Coarse-Grained Models of Proteins: Theory and Applications. , 2011, , 35-83.		12
93	1,4-DHP-lipid parameters and rod like micellae. Journal of Biophysical Chemistry, 2011, 02, 386-394.	0.1	0
94	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.	1.5	36
95	Coarseâ€grained model of nucleic acid bases. Journal of Computational Chemistry, 2010, 31, 1644-1655.	1.5	28
96	Mechanism of formation of the Câ€terminal Î²â€hairpin of the B3 domain of the immunoglobulin binding protein G from Streptococcus. III. Dynamics of longâ€range hydrophobic interactions. Proteins: Structure, Function and Bioinformatics, 2010, 78, 723-737.	1.5	9
97	Potential of Mean Force of Association of Large Hydrophobic Particles: Toward the Nanoscale Limit. Journal of Physical Chemistry B, 2010, 114, 993-1003.	1.2	79
98	Î²-hairpin-forming peptides; models of early stages of protein folding. Biophysical Chemistry, 2010, 151, 1-9.	1.5	65
99	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.	1.5	15
100	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.	1.2	17
101	Towards Temperature Dependent Coarse-grained Potential of Side-chain Interactions for Protein Folding Simulations. , 2010, , .		3
102	Investigation of Protein Folding by Coarse-Grained Molecular Dynamics with the UNRES Force Field. Journal of Physical Chemistry A, 2010, 114, 4471-4485.	1.1	91
103	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.	2.3	46
104	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.	6.6	31
105	Relation between Free Energy Landscapes of Proteins and Dynamics. Journal of Chemical Theory and Computation, 2010, 6, 583-595.	2.3	132
106	Combination of SAXS and NMR Techniques as a Tool for the Determination of Peptide Structure in Solution. Journal of Physical Chemistry Letters, 2010, 1, 3128-3131.	2.1	6
107	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.	2.0	87
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.	1.0	20

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109	How Adequate are One- and Two-Dimensional Free Energy Landscapes for Protein Folding Dynamics?. Physical Review Letters, 2009, 102, 238102.	2.9	48
110	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.	1.5	64
111	Conformational studies of the Câ€terminal 16â€aminoâ€acidâ€residue fragment of the B3 domain of the immunoglobulin binding protein G from Streptococcus. Biopolymers, 2009, 91, 37-51.	1.2	13
112	The role of the Val57 aminoâ€acid residue in the hinge loop of the human cystatin C. Conformational studies of the beta2â€L1â€beta3 segments of wildâ€type human cystatin C and its mutants. Biopolymers, 2009, 91, 373-383.	1.2	24
113	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.	1.5	23
114	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.	1.5	18
115	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.	2.3	93
116	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.	1.2	42
117	Principal Component Analysis for Protein Folding Dynamics. Journal of Molecular Biology, 2009, 385, 312-329.	2.0	331
118	A united residue force-field for calcium-protein interactions. Protein Science, 2009, 13, 2725-2735.	3.1	22
119	Dynamics study on single and multiple Î²-sheets. Advances in Experimental Medicine and Biology, 2009, 611, 293-294.	0.8	0
120	Acidicâ€basic properties of three alanineâ€based peptides containing acidic and basic side chains: Comparison between theory and experiment. Biopolymers, 2008, 90, 724-732.	1.2	18
121	Conformational studies of the Î±â€helical 28â€“43 fragment of the B3 domain of the immunoglobulin binding protein G from Streptococcus. Biopolymers, 2008, 89, 1032-1044.	1.2	10
122	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.	1.2	18
123	Computational techniques for efficient conformational sampling of proteins. Current Opinion in Structural Biology, 2008, 18, 134-139.	2.6	170
124	Implementation of a Serial Replica Exchange Method in a Physics-Based United-Residue (UNRES) Force Field. Journal of Chemical Theory and Computation, 2008, 4, 1386-1400.	2.3	7
125	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.	1.2	36
126	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.	1.2	38

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127	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
128	Simulation of Protein Structure and Dynamics with the Coarse-Grained UNRES Force Field. , 2008, , 107-122.		4
129	Global Optimization in Protein Folding. , 2008, , 1392-1411.		0
130	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.	0.7	19
131	Topology of Type II REases revisited; structural classes and the common conserved core. Nucleic Acids Research, 2007, 35, 2227-2237.	6.5	37
132	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.	1.2	184
133	Protein-Folding Dynamics: Overview of Molecular Simulation Techniques. Annual Review of Physical Chemistry, 2007, 58, 57-83.	4.8	329
134	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.	1.2	27
135	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.	1.2	21
136	Theoretical Study of the Energetics of the Reactions of Triplet Dioxygen with Hydroquinone, Semiquinone, and Their Protonated Forms:Â Relation to the Mechanism of Superoxide Generation in the Respiratory Chain. Journal of Physical Chemistry B, 2007, 111, 3543-3549.	1.2	12
137	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.	1.2	33
138	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.	1.2	46
139	Further Evidence for the Absence of Polyproline II Stretch in the XAO Peptide. Biophysical Journal, 2007, 92, 2904-2917.	0.2	51
140	Potential of Mean Force of Hydrophobic Association:â€‰ Dependence on Solute Size. Journal of Physical Chemistry B, 2007, 111, 10765-10774.	1.2	63
141	Separation of time scale and coupling in the motion governed by the coarse-grained and fine degrees of freedom in a polypeptide backbone. Journal of Chemical Physics, 2007, 127, 155103.	1.2	7
142	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.	1.2	16
143	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.	2.0	66
144	Membrane Initiated Gelsolin Amyloid Formation. , 2006, , 698-699.		0

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145	Molecular dynamics study of amyloid formation of two Abl-SH3 domain peptides. Journal of Peptide Science, 2006, 12, 780-789.	0.8	5
146	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.	1.2	40
147	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.	3.3	156
148	Theoretical calculations of homoconjugation equilibrium constants in systems modeling acid-base interactions in side chains of biomolecules using the potential of mean force. Journal of Computational Chemistry, 2005, 26, 235-242.	1.5	8
149	Interplay of charge distribution and conformation in peptides: Comparison of theory and experiment. Biopolymers, 2005, 80, 214-224.	1.2	8
150	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.	3.3	256
151	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.	0.8	18
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