Valerie Daggett

List of Publications by Year
in descending order

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149	11,844	24978	28224
papers	citations	57 h-index	105 g-index

156	156	156	8708
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Amyloid-Î² Oligomers: Multiple Moving Targets. Biophysica, 2022, 2, 91-110.	0.6	17
2	Conserved patterns and interactions in the unfolding transition state across SH3 domain structural homologues. Protein Science, 2021, 30, 391-407.	3.1	6
3	Modulation of post-powerstroke dynamics in myosin II by 2â€²-deoxy-ADP. Archives of Biochemistry and Biophysics, 2021, 699, 108733.	1.4	6
4	Edge Strand Dissociation and Conformational Changes in Transthyretin under Amyloidogenic Conditions. Biophysical Journal, 2020, 119, 1995-2009.	0.2	12
5	Tumorigenic p53 mutants undergo common structural disruptions including conversion to Î±â€sheet structure. Protein Science, 2020, 29, 1983-1999.	3.1	3
6	Myosin dynamics during relaxation in mouse soleus muscle and modulation by 2â€²â€deoxyâ€ATP. Journal of Physiology, 2020, 598, 5165-5182.	1.3	23
7	Drivers of Î±-Sheet Formation in Transthyretin under Amyloidogenic Conditions. Biochemistry, 2019, 58, 4408-4423.	1.2	12
8	Cardiac myosin activation with 2-deoxy-ATP via increased electrostatic interactions with actin. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 11502-11507.	3.3	30
9	Î±-Sheet secondary structure in amyloid Î²-peptide drives aggregation and toxicity in Alzheimerâ€™s disease. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 8895-8900.	3.3	118
10	Visualizing Protein Folding and Unfolding. Journal of Molecular Biology, 2019, 431, 1540-1564.	2.0	32
11	Shared unfolding pathways of unrelated immunoglobulin-like Î²-sandwich proteins. Protein Engineering, Design and Selection, 2019, 32, 331-345.	1.0	1
12	Chemical and Physical Variability in Structural Isomers of an <scp>l</scp>/<scp>d</scp> Î±-Sheet Peptide Designed To Inhibit Amyloidogenesis. Biochemistry, 2018, 57, 507-510.	1.2	24
13	Protein Folding: Molecular Dynamics Simulations. , 2018, , 1-9.		0
14	Molecular dynamics-derived rotamer libraries for <scp>d</scp>-amino acids within homochiral and heterochiral polypeptides. Protein Engineering, Design and Selection, 2018, 31, 191-204.	1.0	6
15	Protein Engineering Reveals Mechanisms of Functional Amyloid Formation in Pseudomonas aeruginosa Biofilms. Journal of Molecular Biology, 2018, 430, 3751-3763.	2.0	44
16	De Novo Designed Î±-Sheet Peptides Inhibit Functional Amyloid Formation of Streptococcus mutans Biofilms. Journal of Molecular Biology, 2018, 430, 3764-3773.	2.0	21
17	A Carboxylate to Amide Substitution That Switches Protein Folds. Angewandte Chemie, 2018, 130, 12977-12980.	1.6	0
18	A Carboxylate to Amide Substitution That Switches Protein Folds. Angewandte Chemie - International Edition, 2018, 57, 12795-12798.	7.2	4

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19	Validating Molecular Dynamics Simulations against Experimental Observables in Light of Underlying Conformational Ensembles. Journal of Physical Chemistry B, 2018, 122, 6673-6689.	1.2	71
20	The Role of Î±-sheet in Amyloid Oligomer Aggregation and Toxicity. Yale Journal of Biology and Medicine, 2018, 91, 247-255.	0.2	9
21	Molecular mechanisms underlying deoxyâ€ADP.Pi activation of preâ€powerstroke myosin. Protein Science, 2017, 26, 749-762.	3.1	9
22	Insights from molecular dynamics simulations for computational protein design. Molecular Systems Design and Engineering, 2017, 2, 9-33.	1.7	149
23	Simulations of membraneâ€bound diglycosylated human prion protein reveal potential protective mechanisms against misfolding. Journal of Neurochemistry, 2017, 142, 171-182.	2.1	10
24	The Dynameomics Entropy Dictionary: A Large-Scale Assessment of Conformational Entropy across Protein Fold Space. Journal of Physical Chemistry B, 2017, 121, 3933-3945.	1.2	21
25	Designed Î±-sheet peptides suppress amyloid formation in Staphylococcus aureus biofilms. Npj Biofilms and Microbiomes, 2017, 3, 16.	2.9	34
26	Structural and functional diversity among amyloid proteins: Agents of disease, building blocks of biology, and implications for molecular engineering. Biotechnology and Bioengineering, 2017, 114, 7-20.	1.7	27
27	Anin silicoalgorithm for identifying stabilizing pockets in proteins: test case, the Y220C mutant of the p53 tumor suppressor protein. Protein Engineering, Design and Selection, 2016, 29, 377-390.	1.0	13
28	The effect of chirality and steric hindrance on intrinsic backbone conformational propensities: tools for protein design. Protein Engineering, Design and Selection, 2016, 29, 271-280.	1.0	18
29	Insights into Unfolded Proteins from the Intrinsic Ï•/Ïˆ Propensities of the AAXAA Host-Guest Series. Biophysical Journal, 2016, 110, 348-361.	0.2	12
30	Peptides Composed of Alternating L- and D-Amino Acids Inhibit Amyloidogenesis in Three Distinct Amyloid Systems Independent of Sequence. Journal of Molecular Biology, 2016, 428, 2317-2328.	2.0	50
31	New Dynamic Rotamer Libraries: Data-Driven Analysis of Side-Chain Conformational Propensities. Structure, 2016, 24, 187-199.	1.6	45
32	Dynameomics: Dataâ€driven methods and models for utilizing largeâ€scale protein structure repositories for improving fragmentâ€based loop prediction. Protein Science, 2014, 23, 1584-1595.	3.1	8
33	Different misfolding mechanisms converge on common conformational changes. Prion, 2014, 8, 125-135.	0.9	14
34	Molecular Dynamics Simulations Capture the Misfolding of the Bovine Prion Protein at Acidic pH. Biomolecules, 2014, 4, 181-201.	1.8	25
35	DIVE: a data intensive visualization engine. Bioinformatics, 2014, 30, 593-595.	1.8	12
36	Structural and Dynamic Properties of the Human Prion Protein. Biophysical Journal, 2014, 106, 1152-1163.	0.2	31

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37	DIVE: A Graph-Based Visual-Analytics Framework for Big Data. IEEE Computer Graphics and Applications, 2014, 34, 26-37.	1.0	34
38	Nature versus design: the conformational propensities of d-amino acids and the importance of side chain chirality. Protein Engineering, Design and Selection, 2014, 27, 447-455.	1.0	31
39	Designed Î±-sheet peptides inhibit amyloid formation by targeting toxic oligomers. ELife, 2014, 3, e01681.	2.8	67
40	Designed Trpzip-3 Î²-Hairpin Inhibits Amyloid Formation in Two Different Amyloid Systems. ACS Medicinal Chemistry Letters, 2013, 4, 824-828.	1.3	24
41	Using simulations to provide the framework for experimental protein folding studies. Archives of Biochemistry and Biophysics, 2013, 531, 128-135.	1.4	53
42	Structural Consequences of Mutations to the Î±-Tocopherol Transfer Protein Associated with the Neurodegenerative Disease Ataxia with Vitamin E Deficiency. Biochemistry, 2013, 52, 4264-4273.	1.2	23
43	Early steps in thermal unfolding of superoxide dismutase 1 are similar to the conformational changes associated with the ALS-associated A4V mutation. Protein Engineering, Design and Selection, 2013, 26, 503-513.	1.0	24
44	Disruption of the X-loop turn of the prion protein linked to scrapie resistance. Protein Engineering, Design and Selection, 2012, 25, 243-249.	1.0	9
45	A CHEMICAL GROUP GRAPH REPRESENTATION FOR EFFICIENT HIGH-THROUGHPUT ANALYSIS OF ATOMISTIC PROTEIN SIMULATIONS. Journal of Bioinformatics and Computational Biology, 2012, 10, 1250008.	0.3	21
46	Multimolecule test-tube simulations of protein unfolding and aggregation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 17851-17856.	3.3	14
47	When a domain is not a domain, and why it is important to properly filter proteins in databases. BioEssays, 2012, 34, 1060-1069.	1.2	6
48	Protein simulation data in the relational model. Journal of Supercomputing, 2012, 62, 150-173.	2.4	10
49	WAVELET ANALYSIS OF PROTEIN MOTION. International Journal of Wavelets, Multiresolution and Information Processing, 2012, 10, 1250040.	0.9	11
50	Understanding protein unfolding from molecular simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 405-423.	6.2	29
51	A Comparison of Multiscale Methods for the Analysis of Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 8722-8731.	1.2	81
52	Structural Effects of the L145Q, V157F, and R282W Cancer-Associated Mutations in the p53 DNA-Binding Core Domain. Biochemistry, 2011, 50, 5345-5353.	1.2	35
53	Manifestations of Native Topology in the Denatured State Ensemble of Rhodopseudomonas palustris Cytochrome câ€². Biochemistry, 2011, 50, 1029-1041.	1.2	19
54	Protein folds and protein folding. Protein Engineering, Design and Selection, 2011, 24, 11-19.	1.0	59

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55	Implementation of 3D spatial indexing and compression in a large-scale molecular dynamics simulation database for rapid atomic contact detection. BMC Bioinformatics, 2011, 12, 334.	1.2	4
56	The dynameomics rotamer library: Amino acid side chain conformations and dynamics from comprehensive molecular dynamics simulations in water. Protein Science, 2011, 20, 341-352.	3.1	100
57	Generation of a consensus protein domain dictionary. Bioinformatics, 2011, 27, 46-54.	1.8	33
58	The Denatured State Dictates the Topology of Two Proteins with Almost Identical Sequence but Different Native Structure and Function. Journal of Biological Chemistry, 2011, 286, 3863-3872.	1.6	37
59	Introduction to special issue 'Three Decades of Protein Engineering: Impact on Structural Biology and Therapy'. Protein Engineering, Design and Selection, 2011, 24, 1-1.	1.0	1
60	Molecular Dynamics as an Approach to Study Prion Protein Misfolding and the Effect of Pathogenic Mutations. Topics in Current Chemistry, 2011, 305, 169-197.	4.0	24
61	Diverse Effects on the Native Î²-Sheet of the Human Prion Protein Due to Disease-Associated Mutations. Biochemistry, 2010, 49, 9874-9881.	1.2	38
62	Dynameomics: A Comprehensive Database of Protein Dynamics. Structure, 2010, 18, 423-435.	1.6	131
63	Polymorphisms and disease: hotspots of inactivation in methyltransferases. Trends in Biochemical Sciences, 2010, 35, 531-538.	3.7	9
64	Temperature dependence of the flexibility of thermophilic and mesophilic flavoenzymes of the nitroreductase fold. Protein Engineering, Design and Selection, 2010, 23, 327-336.	1.0	36
65	A Comprehensive Multidimensional-Embedded, One-Dimensional Reaction Coordinate for Protein Unfolding/Folding. Biophysical Journal, 2010, 98, 2671-2681.	0.2	24
66	Refolding the Engrailed Homeodomain: Structural Basis for the Accumulation of a Folding Intermediate. Biophysical Journal, 2010, 99, 1628-1636.	0.2	23
67	Influence of pH on the Human Prion Protein: Insights into the Early Steps ofÂMisfolding. Biophysical Journal, 2010, 99, 2289-2298.	0.2	75
68	Pathogenic Mutations in the Hydrophobic Core of the Human Prion Protein Can Promote Structural Instability and Misfolding. Journal of Molecular Biology, 2010, 404, 732-748.	2.0	99
69	The consequences of pathogenic mutations to the human prion protein. Protein Engineering, Design and Selection, 2009, 22, 461-468.	1.0	73
70	Characterization of cellâ€surface prion protein relative to its recombinant analogue: insights from molecular dynamics simulations of diglycosylated, membraneâ€bound human prion protein. Journal of Neurochemistry, 2009, 109, 60-73.	2.1	35
71	Structural Changes to Monomeric CuZn Superoxide Dismutase Caused by the Familial Amyotrophic Lateral Sclerosis-Associated Mutation A4V. Biophysical Journal, 2009, 97, 1709-1718.	0.2	66
72	Dynameomics: A Consensus View of the Protein Unfolding/Folding Transition State Ensemble across a Diverse Set of Protein Folds. Biophysical Journal, 2009, 97, 2958-2966.	0.2	25

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73	A consensus view of fold space: Combining SCOP, CATH, and the Dali Domain Dictionary. Protein Science, 2009, 12, 2150-2160.	3.1	121
74	Species variation in PrPSc protofibril models. Journal of Materials Science, 2008, 43, 3625-3637.	1.7	12
75	Combining experiment and simulation in protein folding: closing the gap for small model systems. Current Opinion in Structural Biology, 2008, 18, 4-9.	2.6	98
76	Side-Chain Dynamics Are Critical for Water Permeation through Aquaporin-1. Biophysical Journal, 2008, 95, 1089-1098.	0.2	28
77	Dynameomics: Largeâ€scale assessment of native protein flexibility. Protein Science, 2008, 17, 2038-2050.	3.1	61
78	Microscopic Reversibility of Protein Folding in Molecular Dynamics Simulations of the Engrailed Homeodomain. Biochemistry, 2008, 47, 7079-7089.	1.2	55
79	Different disease-causing mutations in transthyretin trigger the same conformational conversion. Protein Engineering, Design and Selection, 2008, 21, 187-195.	1.0	20
80	Dynameomics: mass annotation of protein dynamics and unfolding in water by high-throughput atomistic molecular dynamics simulations. Protein Engineering, Design and Selection, 2008, 21, 353-368.	1.0	60
81	Dynameomics: design of a computational lab workflow and scientific data repository for protein simulations. Protein Engineering, Design and Selection, 2008, 21, 369-377.	1.0	41
82	Dynameomics: a multi-dimensional analysis-optimized database for dynamic protein data. Protein Engineering, Design and Selection, 2008, 21, 379-386.	1.0	38
83	The intrinsic conformational propensities of the 20 naturally occurring amino acids and reflection of these propensities in proteins. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 12259-12264.	3.3	120
84	Conformational entropy of alanine versus glycine in protein denatured states. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 2661-2666.	3.3	94
85	Direct Observation of Microscopic Reversibility in Single-molecule Protein Folding. Journal of Molecular Biology, 2007, 366, 677-686.	2.0	58
86	Molecular Mechanism for Low pH Triggered Misfolding of the Human Prion Proteinâ€. Biochemistry, 2007, 46, 3045-3054.	1.2	78
87	Folding Mechanisms of Proteins with High Sequence Identity but Different Foldsâ€. Biochemistry, 2007, 46, 1545-1556.	1.2	23
88	A One-Dimensional Reaction Coordinate for Identification of Transition States from Explicit Solvent Pfold-Like Calculations. Biophysical Journal, 2007, 93, 3382-3391.	0.2	25
89	The role of the turn in Î²â€hairpin formation during WW domain folding. Protein Science, 2007, 16, 2233-2239.	3.1	39
90	Importance of Context in Protein Folding:Â Secondary Structural Propensities versus Tertiary Contact-Assisted Secondary Structure Formationâ€. Biochemistry, 2006, 45, 4153-4163.	1.2	22

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91	Protein Foldingâ^'Simulation. Chemical Reviews, 2006, 106, 1898-1916.	23.0	191
92	The 108M Polymorph of Human Catechol O-Methyltransferase Is Prone to Deformation at Physiological Temperatures. Biochemistry, 2006, 45, 2178-2188.	1.2	23
93	Structural Properties of Prion Protein Protofibrils and Fibrils:Â An Experimental Assessment of Atomic Modelsâ€. Biochemistry, 2006, 45, 15573-15582.	1.2	67
94	Î±-Sheet:â€‰ The Toxic Conformer in Amyloid Diseases?. Accounts of Chemical Research, 2006, 39, 594-602.	7.6	96
95	The Folding Pathway of Spectrin R17 from Experiment and Simulation: Using Experimentally Validated MD Simulations to Characterize States Hinted at by Experiment. Journal of Molecular Biology, 2006, 359, 159-173.	2.0	50
96	Î¦-Analysis at the Experimental Limits: Mechanism of Î²-Hairpin Formation. Journal of Molecular Biology, 2006, 360, 865-881.	2.0	94
97	Ensemble versus single-molecule protein unfolding. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 13445-13450.	3.3	78
98	Characterization of a possible amyloidogenic precursor in glutamine-repeat neurodegenerative diseases. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 13433-13438.	3.3	73
99	Characterization of Two Distinct Î²2-Microglobulin Unfolding Intermediates that May Lead to Amyloid Fibrils of Different Morphologyâ€. Biochemistry, 2005, 44, 16098-16107.	1.2	38
100	Cutoff Size Need Not Strongly Influence Molecular Dynamics Results for Solvated Polypeptides. Biochemistry, 2005, 44, 609-616.	1.2	140
101	Simulation and Experiment Conspire to Reveal Cryptic Intermediates and a Slide from the Nucleation-condensation to Framework Mechanism of Folding. Journal of Molecular Biology, 2005, 350, 757-775.	2.0	62
102	Local environmental effects on the structure of the prion protein. Comptes Rendus - Biologies, 2005, 328, 847-862.	0.1	45
103	Sensitivity of the folding/unfolding transition state ensemble of chymotrypsin inhibitor 2 to changes in temperature and solvent. Protein Science, 2005, 14, 1242-1252.	3.1	46
104	Pauling and Corey's Â-pleated sheet structure may define the prefibrillar amyloidogenic intermediate in amyloid disease. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 11622-11627.	3.3	133
105	Demonstration of a low-energy on-pathway intermediate in a fast-folding protein by kinetics, protein engineering, and simulation. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 6450-6455.	3.3	98
106	From conversion to aggregation: Protofibril formation of the prion protein. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 2293-2298.	3.3	293
107	Anatomy of an Amyloidogenic Intermediate. Structure, 2004, 12, 1847-1863.	1.6	81
108	The Early Steps in the Unfolding of Azurinâ€. Biochemistry, 2004, 43, 15604-15609.	1.2	25

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109	Counteraction of urea-induced protein denaturation by trimethylamine N-oxide: A chemical chaperone at atomic resolution. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 6433-6438.	3.3	291
110	Methods for molecular dynamics simulations of protein folding/unfolding in solution. Methods, 2004, 34, 112-120.	1.9	184
111	Diffusing and Colliding: The Atomic Level Folding/Unfolding Pathway of a Small Helical Protein. Journal of Molecular Biology, 2004, 341, 1109-1124.	2.0	38
112	Is there a unifying mechanism for protein folding?. Trends in Biochemical Sciences, 2003, 28, 18-25.	3.7	420
113	The complete folding pathway of a protein from nanoseconds to microseconds. Nature, 2003, 421, 863-867.	13.7	449
114	The present view of the mechanism of protein folding. Nature Reviews Molecular Cell Biology, 2003, 4, 497-502.	16.1	366
115	Unifying features in protein-folding mechanisms. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 13286-13291.	3.3	225
116	The molecular basis for the chemical denaturation of proteins by urea. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 5142-5147.	3.3	728
117	Simulations of biomolecules: characterization of the early steps in the pH-induced conformational conversion of the hamster, bovine and human forms of the prion protein. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2002, 360, 1165-1178.	1.6	47
118	Protein Folding and Unfolding at Atomic Resolution. Cell, 2002, 108, 573-582.	13.5	467
119	Increasing Temperature Accelerates Protein Unfolding Without Changing the Pathway of Unfolding. Journal of Molecular Biology, 2002, 322, 189-203.	2.0	320
120	Molecular Dynamics Simulations of the Protein Unfolding/Folding Reaction. Accounts of Chemical Research, 2002, 35, 422-429.	7.6	151
121	A microscopic view of peptide and protein solvation. Biophysical Chemistry, 2002, 100, 221-237.	1.5	43
122	Direct Comparison of Experimental and Calculated Folding Free Energies for Hydrophobic Deletion Mutants of Chymotrypsin Inhibitor 2:Â Free Energy Perturbation Calculations Using Transition and Denatured States from Molecular Dynamics Simulations of Unfoldingâ€. Biochemistry, 2001, 40, 2723-2731.	1.2	41
123	A comparison of experimental and computational methods for mapping the interactions present in the transition state for folding of FKBP12. Journal of Biological Physics, 2001, 27, 99-117.	0.7	4
124	Validation of protein-unfolding transition states identified in molecular dynamics simulations. Biochemical Society Symposia, 2001, 68, 83-93.	2.7	1
125	Characterization of the unfolding pathway of the cell-cycle protein p13suc1 by molecular dynamics simulations: implications for domain swapping. Structure, 2000, 8, 101-110.	1.6	34
126	The effects of disulfide bonds on the denatured state of barnase. Protein Science, 2000, 9, 2394-2404.	3.1	51

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127	Towards a complete description of the structural and dynamic properties of the denatured state of barnase and the role of residual structure in folding 1 1Edited by B. Honig. Journal of Molecular Biology, 2000, 296, 1257-1282.	2.0	171
128	NMR Studies of the Association of Cytochromeb5with Cytochromecâ€. Biochemistry, 2000, 39, 14025-14039.	1.2	20
129	Engineering Out Motion:â€‰ Introduction of a de Novo Disulfide Bond and a Salt Bridge Designed To Close a Dynamic Cleft on the Surface of Cytochrome b5. Biochemistry, 1999, 38, 5054-5064.	1.2	21
130	Engineering Out Motion:â€‰ A Surface Disulfide Bond Alters the Mobility of Tryptophan 22 in Cytochrome b5 As Probed by Time-Resolved Fluorescence and 1H NMR Experiments. Biochemistry, 1999, 38, 5065-5075.	1.2	18
131	Analysis methods for comparison of multiple molecular dynamics trajectories: applications to protein unfolding pathways and denatured ensembles 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 1999, 290, 283-304.	2.0	62
132	PrP^cGlycoform Heterogeneity as a Function of Brain Region: Implications for Selective Targeting of Neurons by Prion Strains. Journal of Neuropathology and Experimental Neurology, 1999, 58, 1000-1009.	0.9	103
133	Conformational search using a molecular dynamics-minimization procedure: Applications to clusters of coulombic charges, Lennard-Jones particles, and waters. Journal of Computational Chemistry, 1998, 19, 60-70.	1.5	12
134	Molecular dynamics simulations of hydrophobic collapse of ubiquitin. Protein Science, 1998, 7, 860-874.	3.1	85
135	Combined Molecular Dynamics and Î¦-Value Analysis of Structureâ^'Reactivity Relationships in the Transition State and Unfolding Pathway of Barnase:Â Structural Basis of Hammond and Anti-Hammond Effects. Journal of the American Chemical Society, 1998, 120, 12740-12754.	6.6	67
136	Barstar Has a Highly Dynamic Hydrophobic Core:Â Evidence from Molecular Dynamics Simulations and Nuclear Magnetic Resonance Relaxation Dataâ€. Biochemistry, 1998, 37, 11182-11192.	1.2	65
137	Molecular dynamics simulation of the unfolding of barnase: characterization of the major intermediate 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 1998, 275, 677-694.	2.0	114
138	Non-native interactions in protein folding intermediates: molecular dynamics simulations of hen lysozyme. Journal of Molecular Biology, 1998, 284, 793-806.	2.0	48
139	Selective Neuronal Targeting in Prion Disease. Neuron, 1997, 19, 1337-1348.	3.8	199
140	Calibration and Testing of a Water Model for Simulation of the Molecular Dynamics of Proteins and Nucleic Acids in Solution. Journal of Physical Chemistry B, 1997, 101, 5051-5061.	1.2	503
141	Identification and Characterization of the Unfolding Transition State of Chymotrypsin Inhibitor 2 by Molecular Dynamics Simulations. Journal of Molecular Biology, 1996, 257, 412-429.	2.0	236
142	Structure of the Transition State for Folding of a Protein Derived from Experiment and Simulation. Journal of Molecular Biology, 1996, 257, 430-440.	2.0	227
143	Testing the Modified Hydration-Shell Hydrogen-Bond Model of Hydrophobic Effects Using Molecular Dynamics Simulation. The Journal of Physical Chemistry, 1996, 100, 5616-5619.	2.9	56
144	Potential energy function and parameters for simulations of the molecular dynamics of proteins and nucleic acids in solution. Computer Physics Communications, 1995, 91, 215-231.	3.0	431

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145	Investigation of the solution structure of chymotrypsin inhibitor 2 using molecular dynamics: comparison to X-ray crystallographic and NMR data. Protein Engineering, Design and Selection, 1995, 8, 1117-1128.	1.0	39
146	Molecular Dynamics Simulation of Cytochrome b5: Implications for Protein-Protein Recognition. Biochemistry, 1995, 34, 9682-9693.	1.2	66
147	Molecular Dynamics Simulations of Protein Unfolding and Limited Refolding: Characterization of Partially Unfolded States of Ubiquitin in 60% Methanol and in Water. Journal of Molecular Biology, 1995, 247, 501-520.	2.0	102
148	Protein Unfolding Pathways Explored Through Molecular Dynamics Simulations. Journal of Molecular Biology, 1993, 232, 600-619.	2.0	178
149	Molecular dynamics simulations of helix denaturation. Journal of Molecular Biology, 1992, 223, 1121-1138.	2.0	231