Yong Duan

List of Publications by Year in descending order

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95 papers	14,216 citations	87723 38 h-index	45213 90 g-index
95 all docs	95 docs citations	95 times ranked	14434 citing authors

#	Article	IF	Citations
1	Calculating Structures and Free Energies of Complex Molecules:â€‰ Combining Molecular Mechanics and Continuum Models. Accounts of Chemical Research, 2000, 33, 889-897.	7.6	4,098
2	A point-charge force field for molecular mechanics simulations of proteins based on condensed-phase quantum mechanical calculations. Journal of Computational Chemistry, 2003, 24, 1999-2012.	1.5	4,028
3	Pathways to a Protein Folding Intermediate Observed in a 1-Microsecond Simulation in Aqueous Solution. , 1998, 282, 740-744.		1,188
4	Distinguish protein decoys by Using a scoring function based on a new AMBER force field, short molecular dynamics simulations, and the generalized born solvent model. Proteins: Structure, Function and Bioinformatics, 2004, 55, 620-634.	1.5	256
5	Molecular dynamics and free-energy calculations applied to affinity maturation in antibody 48G7. Proceedings of the National Academy of Sciences of the United States of America, 1999, 96, 14330-14335.	3.3	252
6	Polarization effects in molecular mechanical force fields. Journal of Physics Condensed Matter, 2009, 21, 333102.	0.7	236
7	Folding free-energy landscape of villin headpiece subdomain from molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 4925-4930.	3.3	217
8	Use of MM-PB/SA in estimating the free energies of proteins: Application to native, intermediates, and unfolded villin headpiece. Proteins: Structure, Function and Bioinformatics, 2000, 39, 309-316.	1.5	179
9	New-Generation Amber United-Atom Force Field. Journal of Physical Chemistry B, 2006, 110, 13166-13176.	1.2	176
10	Dual Binding Modes of Congo Red to Amyloid Protofibril Surface Observed in Molecular Dynamics Simulations. Journal of the American Chemical Society, 2007, 129, 1225-1232.	6.6	163
11	Strike a balance: Optimization of backbone torsion parameters of AMBER polarizable force field for simulations of proteins and peptides. Journal of Computational Chemistry, 2006, 27, 781-790.	1.5	159
12	Ab initio Folding Simulation of the Trp-cage Mini-protein Approaches NMR Resolution. Journal of Molecular Biology, 2003, 327, 711-717.	2.0	157
13	The early stage of folding of villin headpiece subdomain observed in a 200-nanosecond fully solvated molecular dynamics simulation. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 9897-9902.	3.3	147
14	Development of Polarizable Models for Molecular Mechanical Calculations I: Parameterization of Atomic Polarizability. Journal of Physical Chemistry B, 2011, 115, 3091-3099.	1.2	137
15	The Binding of Thioflavin T and Its Neutral Analog BTA-1 to Protofibrils of the Alzheimerâ€™s Disease Aî²16â€“22 Peptide Probed by Molecular Dynamics Simulations. Journal of Molecular Biology, 2008, 384, 718-729.	2.0	132
16	Development of Polarizable Models for Molecular Mechanical Calculations II: Induced Dipole Models Significantly Improve Accuracy of Intermolecular Interaction Energies. Journal of Physical Chemistry B, 2011, 115, 3100-3111.	1.2	116
17	Solvation effects on alanine dipeptide: A MP2/cc-pVTZ//MP2/6-31G** study of (?, ?) energy maps and conformers in the gas phase, ether, and water. Journal of Computational Chemistry, 2004, 25, 1699-1716.	1.5	114
18	Improved sampling methods for molecular simulation. Current Opinion in Structural Biology, 2007, 17, 187-191.	2.6	110

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19	Convergence of replica exchange molecular dynamics. Journal of Chemical Physics, 2005, 123, 154105.	1.2	107
20	Molecular dynamics simulation study of DNA dodecamer d(CGCGAATTCGCG) in solution: conformation and hydration. Journal of Molecular Biology, 1997, 272, 553-572.	2.0	100
21	Ligand Entry and Exit Pathways in the Î²2-Adrenergic Receptor. Journal of Molecular Biology, 2009, 392, 1102-1115.	2.0	94
22	Concerted Perturbation Observed in a Hub Network in Alzheimerâ€™s Disease. PLoS ONE, 2012, 7, e40498.	1.1	91
23	Multiple Roles of a Conserved GAF Domain Tyrosine Residue in Cyanobacterial and Plant Phytochromesâ€. Biochemistry, 2005, 44, 15203-15215.	1.2	89
24	Two-stage Folding of HP-35 from Ab Initio Simulations. Journal of Molecular Biology, 2007, 370, 196-206.	2.0	83
25	Elongation of Ordered Peptide Aggregate of an Amyloidogenic Hexapeptide NFGAIL Observed in Molecular Dynamics Simulations with Explicit Solvent. Journal of the American Chemical Society, 2005, 127, 13530-13537.	6.6	77
26	Chromophore Channeling in the G-Protein Coupled Receptor Rhodopsin. Journal of the American Chemical Society, 2007, 129, 6970-6971.	6.6	69
27	Statistical characterization of salt bridges in proteins. Proteins: Structure, Function and Bioinformatics, 2005, 60, 732-739.	1.5	66
28	Phenol Red Interacts with the Protofibril-Like Oligomers of an Amyloidogenic Hexapeptide NFGAIL through Both Hydrophobic and Aromatic Contacts. Biophysical Journal, 2006, 91, 3664-3672.	0.2	61
29	The Role of Phe in the Formation of Well-Ordered Oligomers of Amyloidogenic Hexapeptide (NFGAIL) Observed in Molecular Dynamics Simulations with Explicit Solvent. Biophysical Journal, 2005, 88, 2897-2906.	0.2	60
30	Development of Polarizable Models for Molecular Mechanical Calculations. 4. van der Waals Parametrization. Journal of Physical Chemistry B, 2012, 116, 7088-7101.	1.2	60
31	Characterizing the Rate-Limiting Step of Trp-Cage Folding by All-Atom Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2004, 108, 13855-13865.	1.2	59
32	Large-Scale Conformational Dynamics of the HIV-1 Integrase Core Domain and Its Catalytic Loop Mutants. Biophysical Journal, 2005, 88, 3133-3146.	0.2	58
33	Formation of Partially Ordered Oligomers of Amyloidogenic Hexapeptide (NFGAIL) in Aqueous Solution Observed in Molecular Dynamics Simulations. Biophysical Journal, 2004, 87, 3000-3009.	0.2	57
34	Breaking non-native hydrophobic clusters is the rate-limiting step in the folding of an alanine-based peptide. Biopolymers, 2003, 68, 63-75.	1.2	55
35	Study of the stability and unfolding mechanism of BBA1 by molecular dynamics simulations at different temperatures. Protein Science, 1999, 8, 1292-1304.	3.1	49
36	Development of Polarizable Models for Molecular Mechanical Calculations. 3. Polarizable Water Models Conforming to Thole Polarization Screening Schemes. Journal of Physical Chemistry B, 2012, 116, 7999-8008.	1.2	49

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37	Trends in template/fragment-free protein structure prediction. Theoretical Chemistry Accounts, 2011, 128, 3-16.	0.5	48
38	Down-Regulation of Energy Metabolism in Alzheimer's Disease is a Protective Response of Neurons to the Microenvironment. Journal of Alzheimer's Disease, 2012, 28, 389-402.	1.2	44
39	Computational protein folding: From lattice to all-atom. IBM Systems Journal, 2001, 40, 297-309.	3.1	40
40	Ab Initio Folding of Albumin Binding Domain from All-Atom Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2007, 111, 5458-5463.	1.2	39
41	Characteristic Transformation of Blood Transcriptome in Alzheimer's Disease. Journal of Alzheimer's Disease, 2013, 35, 373-386.	1.2	36
42	Accurate ab Initio Study on the Hydrogen-Bond Pairs in Protein Secondary Structures. Journal of Chemical Theory and Computation, 2007, 3, 1527-1537.	2.3	35
43	Folding processes of the B domain of protein A to the native state observed in all-atom ab initio folding simulations. Journal of Chemical Physics, 2008, 128, 235105.	1.2	35
44	Deprotonation of D96 in Bacteriorhodopsin Opens the Proton Uptake Pathway. Structure, 2013, 21, 290-297.	1.6	35
45	Fs-21 Peptides Can Form Both Single Helix and Helixâ^'Turnâ^'Helix. Journal of Physical Chemistry B, 2004, 108, 7479-7489.	1.2	34
46	Hidden Risk Genes with High-Order Intragenic Epistasis in Alzheimer's Disease. Journal of Alzheimer's Disease, 2014, 41, 1039-1056.	1.2	34
47	Effects of Posttranslational Modifications on the Structure and Dynamics of Histone H3 N-Terminal Peptide. Biophysical Journal, 2008, 94, 4579-4585.	0.2	33
48	Retinal release from opsin in molecular dynamics simulations. Journal of Molecular Recognition, 2011, 24, 350-358.	1.1	33
49	Comparison between Generalized-Born and Poissonâ€"Boltzmann methods in physics-based scoring functions for protein structure prediction. Journal of Molecular Modeling, 2005, 12, 101-110.	0.8	32
50	Molecular Dynamics Simulations and Free Energy Analyses on the Dimer Formation of an Amyloidogenic Heptapeptide from Human Î²2-Microglobulin: Implication for the Protofibril Structure. Journal of Molecular Biology, 2006, 356, 1049-1063.	2.0	28
51	Alzheimer's Disease Drug Candidates Stabilize A-Î² Protein Native Structure by Interacting with the Hydrophobic Core. Biophysical Journal, 2011, 100, 1076-1082.	0.2	27
52	Dynamic Contributions to the DNA Binding Entropy of theEcoRI andEcoRV Restriction Endonucleases. Journal of Molecular Biology, 1996, 264, 546-555.	2.0	26
53	Insights into Ligand Binding to PreQ1 Riboswitch Aptamer from Molecular Dynamics Simulations. PLoS ONE, 2014, 9, e92247.	1.1	26
54	Development of Polarizable Gaussian Model for Molecular Mechanical Calculations I: Atomic Polarizability Parameterization To Reproduce ab Initio Anisotropy. Journal of Chemical Theory and Computation, 2019, 15, 1146-1158.	2.3	26

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55	Denatured-State Ensemble and the Early-Stage Folding of the G29A Mutant of the B-Domain of Protein A. Journal of Physical Chemistry B, 2005, 109, 9073-9081.	1.2	25
56	Binding modes of CCR5-targetting HIV entry inhibitors: Partial and full antagonists. Journal of Molecular Graphics and Modelling, 2008, 26, 1287-1295.	1.3	25
57	The role of plastic Î²-hairpin and weak hydrophobic core in the stability and unfolding of a full sequence design protein. Journal of Chemical Physics, 2004, 121, 12104-12111.	1.2	24
58	The fast-folding HP35 double mutant has a substantially reduced primary folding free energy barrier. Journal of Chemical Physics, 2008, 129, 155104.	1.2	24
59	Probing the stability-limiting regions of an antibody single-chain variable fragment: a molecular dynamics simulation study. Protein Engineering, Design and Selection, 2011, 24, 649-657.	1.0	24
60	Dual folding pathways of an Î±/Îβ protein from all-atom ab initio folding simulations. Journal of Chemical Physics, 2009, 131, 165105.	1.2	22
61	Loop Conformation and Dynamics of the Escherichia coli HPPK Apo-Enzyme and Its Binary Complex with MgATP. Biophysical Journal, 2005, 89, 95-106.	0.2	21
62	Two-Way Effects between Hydrogen Bond and Intramolecular Resonance Effect: An Ab Initio Study on Complexes of Formamide and Its Derivatives with Water. Journal of Physical Chemistry A, 2008, 112, 5436-5447.	1.1	19
63	Efficient formulation of polarizable Gaussian multipole electrostatics for biomolecular simulations. Journal of Chemical Physics, 2020, 153, 114116.	1.2	19
64	Molecular Dynamics Simulations Suggest That TheEcoRI Kink is an Example of Molecular Strain. Journal of Biomolecular Structure and Dynamics, 1994, 12, 487-525.	2.0	17
65	Folding Transition-State and Denatured-State Ensembles of FSD-1 from Folding and Unfolding Simulations. Journal of Physical Chemistry B, 2006, 110, 22001-22008.	1.2	15
66	Grow to Fit Molecular Dynamics (G2FMD): an ab initio method for protein side-chain assignment and refinement. Protein Engineering, Design and Selection, 2006, 19, 55-65.	1.0	15
67	Folding Network of Villin Headpiece Subdomain. Biophysical Journal, 2010, 99, 3374-3384.	0.2	15
68	Robust Gene Dysregulation in Alzheimer's Disease Brains. Journal of Alzheimer's Disease, 2014, 41, 587-597.	1.2	15
69	State of the art in studying protein folding and protein structure prediction using molecular dynamics methods. Journal of Molecular Graphics and Modelling, 2001, 19, 146-149.	1.3	13
70	Cholic acid micellesâ€"controlling the size of the aqueous cavity by PEGylation. Physical Chemistry Chemical Physics, 2010, 12, 1589.	1.3	13
71	The protein folding network indicates that the ultrafast folding mutant of villin headpiece subdomain has a deeper folding funnel. Journal of Chemical Physics, 2011, 134, 205104.	1.2	13
72	Does a diol cyclic urea inhibitor of HIV-1 protease bind tighter than its corresponding alcohol form? A study by free energy perturbation and continuum electrostatics calculations. Journal of Computer-Aided Molecular Design, 2001, 15, 145-156.	1.3	12

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73	PyRESP: A Program for Electrostatic Parameterizations of Additive and Induced Dipole Polarizable Force Fields. Journal of Chemical Theory and Computation, 2022, 18, 3654-3670.	2.3	12
74	Gradient SHAKE: An improved method for constrained energy minimization in macromolecular simulations. Journal of Computational Chemistry, 1995, 16, 1351-1356.	1.5	11
75	Key residues in TLR4-MD2 tetramer formation identified by free energy simulations. PLoS Computational Biology, 2019, 15, e1007228.	1.5	11
76	Stress tensor and constant pressure simulation for polarizable Gaussian multipole model. Journal of Chemical Physics, 2022, 156, 114114.	1.2	10
77	DIRECT INTERACTION ENERGY: A COMPUTATIONAL QUANTITY FOR PARAMETERIZATION OF CONDENSED-PHASE FORCE FIELDS AND ITS APPLICATION TO HYDROGEN BONDING. Journal of Theoretical and Computational Chemistry, 2005, 04, 689-705.	1.8	9
78	Incorporating intermolecular distance into protein-protein docking. Protein Engineering, Design and Selection, 2005, 17, 837-845.	1.0	7
79	iBIG: An Integrative Network Tool for Supporting Human Disease Mechanism Studies. Genomics, Proteomics and Bioinformatics, 2013, 11, 166-171.	3.0	7
80	Schiff Base Switch II Precedes the Retinal Thermal Isomerization in the Photocycle of Bacteriorhodopsin. PLoS ONE, 2013, 8, e69882.	1.1	7
81	Conformational Changes in Protein Function. Methods in Molecular Biology, 2008, 443, 258-275.	0.4	6
82	HIV Co-Receptor CCR5: Structure and Interactions with Inhibitors. Infectious Disorders - Drug Targets, 2009, 9, 279-288.	0.4	6
83	Statistical properties and kinetics of end-end contact formation of unfolded polypeptides: A systematic molecular dynamics study. Journal of Chemical Physics, 2007, 126, 045108.	1.2	5
84	Chromosome 19p in Alzheimer's Disease: When Genome Meets Transcriptome. Journal of Alzheimer's Disease, 2013, 38, 245-250.	1.2	5
85	Conformational Elasticity can Facilitate TALEâ€“DNA Recognition. Advances in Protein Chemistry and Structural Biology, 2014, 94, 347-364.	1.0	5
86	Use of MM-PB/SA in estimating the free energies of proteins: Application to native, intermediates, and unfolded villin headpiece. , 2000, 39, 309.		5
87	Protein Folding and Unfolding by All-Atom Molecular Dynamics Simulations. Methods in Molecular Biology, 2008, 443, 277-295.	0.4	5
88	7 Ã— 7 RMSD matrix: A new method for quantitative comparison of the transmembrane domain structures in the G-protein coupled receptors. Journal of Structural Biology, 2017, 199, 87-101.	1.3	4
89	Functional Networking of Human Divergently Paired Genes (DPGs). PLoS ONE, 2013, 8, e78896.	1.1	3
90	Stable Closure of the Cytoplasmic Half-Channel Is Required for Efficient Proton Transport at Physiological Membrane Potentials in the Bacteriorhodopsin Catalytic Cycle. Biochemistry, 2014, 53, 2380-2390.	1.2	3

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91	Assessment of the transmembrane domain structures in GPCR Dock 2013 models. Journal of Structural Biology, 2018, 201, 210-220.	1.3	1
92	<scp>C1188D</scp> mutation abolishes specific recognition between <scp>MLL1â€CXXC</scp> domain and <scp>CpG</scp> site by inducing conformational switch of flexible Nâ€terminal. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1401-1412.	1.5	1
93	Use of MM-PB/SA in estimating the free energies of proteins: Application to native, intermediates, and unfolded villin headpiece. , 2000, 39, 309.		1
94	Use of MM-PB/SA in estimating the free energies of proteins: Application to native, intermediates, and unfolded villin headpiece. , 2000, 39, 309.		1
95	VERIFICATION OF THE GENERALIZED BORN MODEL AT SHORT DISTANCES. Journal of Mechanics in Medicine and Biology, 2013, 13, 1340020.	0.3	0