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	Stress tensor and constant pressure simulation for polarizable Gaussian multipole model. Journal of Chemical Physics, 2022, 156, 114114.	1.2	10
2	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
3	Efficient formulation of polarizable Gaussian multipole electrostatics for biomolecular simulations. Journal of Chemical Physics, 2020, 153, 114116.	1.2	19
4	<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
5	Key residues in TLR4-MD2 tetramer formation identified by free energy simulations. PLoS Computational Biology, 2019, 15, e1007228.	1.5	11
6	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
7	Assessment of the transmembrane domain structures in GPCR Dock 2013 models. Journal of Structural Biology, 2018, 201, 210-220.	1.3	1
8	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
9	Insights into Ligand Binding to PreQ1 Riboswitch Aptamer from Molecular Dynamics Simulations. PLoS ONE, 2014, 9, e92247.	1.1	26
10	Robust Gene Dysregulation in Alzheimer's Disease Brains. Journal of Alzheimer's Disease, 2014, 41, 587-597.	1.2	15
11	Conformational Elasticity can Facilitate TALEâ€“DNA Recognition. Advances in Protein Chemistry and Structural Biology, 2014, 94, 347-364.	1.0	5
12	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
13	Hidden Risk Genes with High-Order Intragenic Epistasis in Alzheimer's Disease. Journal of Alzheimer's Disease, 2014, 41, 1039-1056.	1.2	34
14	iBIG: An Integrative Network Tool for Supporting Human Disease Mechanism Studies. Genomics, Proteomics and Bioinformatics, 2013, 11, 166-171.	3.0	7
15	Deprotonation of D96 in Bacteriorhodopsin Opens the Proton Uptake Pathway. Structure, 2013, 21, 290-297.	1.6	35
16	VERIFICATION OF THE GENERALIZED BORN MODEL AT SHORT DISTANCES. Journal of Mechanics in Medicine and Biology, 2013, 13, 1340020.	0.3	0
17	Characteristic Transformation of Blood Transcriptome in Alzheimer's Disease. Journal of Alzheimer's Disease, 2013, 35, 373-386.	1.2	36
18	Chromosome 19p in Alzheimer's Disease: When Genome Meets Transcriptome. Journal of Alzheimer's Disease, 2013, 38, 245-250.	1.2	5

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19	Functional Networking of Human Divergently Paired Genes (DPGs). PLoS ONE, 2013, 8, e78896.	1.1	3
20	Schiff Base Switch II Precedes the Retinal Thermal Isomerization in the Photocycle of Bacteriorhodopsin. PLoS ONE, 2013, 8, e69882.	1.1	7
21	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
22	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
23	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
24	Concerted Perturbation Observed in a Hub Network in Alzheimerâ€™s Disease. PLoS ONE, 2012, 7, e40498.	1.1	91
25	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
26	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
27	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
28	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
29	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
30	Trends in template/fragment-free protein structure prediction. Theoretical Chemistry Accounts, 2011, 128, 3-16.	0.5	48
31	Retinal release from opsin in molecular dynamics simulations. Journal of Molecular Recognition, 2011, 24, 350-358.	1.1	33
32	Folding Network of Villin Headpiece Subdomain. Biophysical Journal, 2010, 99, 3374-3384.	0.2	15
33	Cholic acid micellesâ€”controlling the size of the aqueous cavity by PEGylation. Physical Chemistry Chemical Physics, 2010, 12, 1589.	1.3	13
34	Dual folding pathways of an Î±/Î² protein from all-atom ab initio folding simulations. Journal of Chemical Physics, 2009, 131, 165105.	1.2	22
35	Polarization effects in molecular mechanical force fields. Journal of Physics Condensed Matter, 2009, 21, 333102.	0.7	236
36	Ligand Entry and Exit Pathways in the Î²2-Adrenergic Receptor. Journal of Molecular Biology, 2009, 392, 1102-1115.	2.0	94

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37	HIV Co-Receptor CCR5: Structure and Interactions with Inhibitors. Infectious Disorders - Drug Targets, 2009, 9, 279-288.	0.4	6
38	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
39	Effects of Posttranslational Modifications on the Structure and Dynamics of Histone H3 N-Terminal Peptide. Biophysical Journal, 2008, 94, 4579-4585.	0.2	33
40	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
41	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
42	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
43	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
44	Conformational Changes in Protein Function. Methods in Molecular Biology, 2008, 443, 258-275.	0.4	6
45	Protein Folding and Unfolding by All-Atom Molecular Dynamics Simulations. Methods in Molecular Biology, 2008, 443, 277-295.	0.4	5
46	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
47	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
48	Two-stage Folding of HP-35 from Ab Initio Simulations. Journal of Molecular Biology, 2007, 370, 196-206.	2.0	83
49	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
50	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
51	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
52	Chromophore Channeling in the G-Protein Coupled Receptor Rhodopsin. Journal of the American Chemical Society, 2007, 129, 6970-6971.	6.6	69
53	Improved sampling methods for molecular simulation. Current Opinion in Structural Biology, 2007, 17, 187-191.	2.6	110
54	New-Generation Amber United-Atom Force Field. Journal of Physical Chemistry B, 2006, 110, 13166-13176.	1.2	176

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55	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
56	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
57	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
58	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
59	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
60	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
61	Statistical characterization of salt bridges in proteins. Proteins: Structure, Function and Bioinformatics, 2005, 60, 732-739.	1.5	66
62	Incorporating intermolecular distance into protein-protein docking. Protein Engineering, Design and Selection, 2005, 17, 837-845.	1.0	7
63	Convergence of replica exchange molecular dynamics. Journal of Chemical Physics, 2005, 123, 154105.	1.2	107
64	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
65	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
66	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
67	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
68	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
69	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
70	Multiple Roles of a Conserved GAF Domain Tyrosine Residue in Cyanobacterial and Plant Phytochromesâ€. Biochemistry, 2005, 44, 15203-15215.	1.2	89
71	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
72	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

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73	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
74	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
75	Fs-21 Peptides Can Form Both Single Helix and Helixâ^'Turnâ^'Helix. Journal of Physical Chemistry B, 2004, 108, 7479-7489.	1.2	34
76	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
77	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
78	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
79	Ab initio Folding Simulation of the Trp-cage Mini-protein Approaches NMR Resolution. Journal of Molecular Biology, 2003, 327, 711-717.	2.0	157
80	Computational protein folding: From lattice to all-atom. IBM Systems Journal, 2001, 40, 297-309.	3.1	40
81	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
82	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
83	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
84	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
85	Use of MM-PB/SA in estimating the free energies of proteins: Application to native, intermediates, and unfolded villin headpiece. , 2000, 39, 309.		1
86	Use of MM-PB/SA in estimating the free energies of proteins: Application to native, intermediates, and unfolded villin headpiece. , 2000, 39, 309.		1
87	Use of MM-PB/SA in estimating the free energies of proteins: Application to native, intermediates, and unfolded villin headpiece. , 2000, 39, 309.		5
88	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
89	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
90	Pathways to a Protein Folding Intermediate Observed in a 1-Microsecond Simulation in Aqueous Solution. , 1998, 282, 740-744.		1,188

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91	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
92	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
93	Dynamic Contributions to the DNA Binding Entropy of theEcoRI andEcoRV Restriction Endonucleases. Journal of Molecular Biology, 1996, 264, 546-555.	2.0	26
94	Gradient SHAKE: An improved method for constrained energy minimization in macromolecular simulations. Journal of Computational Chemistry, 1995, 16, 1351-1356.	1.5	11
95	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