Donald Hamelberg

List of Publications by Year
in descending order

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93	4,676	159585	102487
papers	citations	30 h-index	66 g-index

106	106	106	4937
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Accelerated molecular dynamics: A promising and efficient simulation method for biomolecules. Journal of Chemical Physics, 2004, 120, 11919-11929.	3.0	1,313
2	Standard Free Energy of Releasing a Localized Water Molecule from the Binding Pockets of Proteins:Â Double-Decoupling Method. Journal of the American Chemical Society, 2004, 126, 7683-7689.	13.7	241
3	Sampling of slow diffusive conformational transitions with accelerated molecular dynamics. Journal of Chemical Physics, 2007, 127, 155102.	3.0	224
4	Dynamical network of residueâ€“residue contacts reveals coupled allosteric effects in recognition, catalysis, and mutation. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 4735-4740.	7.1	138
5	Flexible Structure of DNA:Â Ion Dependence of Minor-Groove Structure and Dynamics. Journal of the American Chemical Society, 2000, 122, 10513-10520.	13.7	117
6	A statistical analysis of the precision of reweighting-based simulations. Journal of Chemical Physics, 2008, 129, 034103.	3.0	113
7	Fast Peptidyl cisâ^'trans Isomerization within the Flexible Gly-Rich Flaps of HIV-1 Protease. Journal of the American Chemical Society, 2005, 127, 13778-13779.	13.7	99
8	Influence of the Dynamic Positions of Cations on the Structure of the DNA Minor Groove:Â Sequence-Dependent Effects. Journal of the American Chemical Society, 2001, 123, 7745-7755.	13.7	95
9	DNA Sequence Dependent Monomerâ^'Dimer Binding Modulation of Asymmetric Benzimidazole Derivatives. Journal of the American Chemical Society, 2004, 126, 143-153.	13.7	95
10	A dry ligand-binding cavity in a solvated protein. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 6296-6301.	7.1	94
11	Phosphorylation Effects on cis/trans Isomerization and the Backbone Conformation of Serineâ^'Proline Motifs:Â Accelerated Molecular Dynamics Analysis. Journal of the American Chemical Society, 2005, 127, 1969-1974.	13.7	89
12	Characterization of a Novel DNA Minor-Groove Complex. Biophysical Journal, 2004, 86, 1028-1041.	0.5	88
13	Protein conformational dynamics in the mechanism of HIV-1 protease catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 20982-20987.	7.1	86
14	Replica-Exchange Accelerated Molecular Dynamics (REXAMD) Applied to Thermodynamic Integration. Journal of Chemical Theory and Computation, 2008, 4, 1565-1569.	5.3	82
15	Reoptimization of the AMBER Force Field Parameters for Peptide Bond (Omega) Torsions Using Accelerated Molecular Dynamics. Journal of Physical Chemistry B, 2009, 113, 16590-16595.	2.6	77
16	Relating kinetic rates and local energetic roughness by accelerated molecular-dynamics simulations. Journal of Chemical Physics, 2005, 122, 241103.	3.0	76
17	Strong Binding in the DNA Minor Groove by an Aromatic Diamidine with a Shape That Does Not Match the Curvature of the Groove. Journal of the American Chemical Society, 2002, 124, 13680-13681.	13.7	71
18	Resolving the complex role of enzyme conformational dynamics in catalytic function. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 5699-5704.	7.1	63

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19	Structural Selectivity of Aromatic Diamidines. Journal of Medicinal Chemistry, 2004, 47, 5729-5742.	6.4	57
20	The folding energy landscape and phosphorylation: modeling the conformational switch of the NFAT regulatory domain. FASEB Journal, 2005, 19, 1389-1395.	0.5	53
21	Mechanistic Insight into the Role of Transition-State Stabilization in Cyclophilin A. Journal of the American Chemical Society, 2009, 131, 147-152.	13.7	53
22	Towards fast, rigorous and efficient conformational sampling of biomolecules: Advances in accelerated molecular dynamics. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 878-888.	2.4	51
23	Coupling Accelerated Molecular Dynamics Methods with Thermodynamic Integration Simulations. Journal of Chemical Theory and Computation, 2008, 4, 1516-1525.	5.3	48
24	The role of conserved water molecules in the catalytic domain of protein kinases. Proteins: Structure, Function and Bioinformatics, 2009, 76, 527-535.	2.6	47
25	A proposed signaling motif for nuclear import in mRNA processing via the formation of arginine claw. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 14947-14951.	7.1	44
26	Deciphering the role of glucosamine-6-phosphate in the riboswitch action of glmS ribozyme. Rna, 2010, 16, 2455-2463.	3.5	44
27	Effect of a neutralized phosphate backbone on the minor groove of B-DNA: molecular dynamics simulation studies. Nucleic Acids Research, 2002, 30, 3615-3623.	14.5	42
28	On the Application of Accelerated Molecular Dynamics to Liquid Water Simulations. Journal of Physical Chemistry B, 2006, 110, 22695-22701.	2.6	40
29	Insight into the role of hydration on protein dynamics. Journal of Chemical Physics, 2006, 125, 094905.	3.0	36
30	Conformational Plasticity of an Enzyme during Catalysis: Intricate Coupling between Cyclophilin A Dynamics and Substrate Turnover. Biophysical Journal, 2013, 104, 216-226.	0.5	36
31	Elucidating Allosteric Communications in Proteins with Difference Contact Network Analysis. Journal of Chemical Information and Modeling, 2018, 58, 1325-1330.	5.4	36
32	Cyclodextrin Complexes of Reduced Bromonoscapine in Guar Gum Microspheres Enhance Colonic Drug Delivery. Molecular Pharmaceutics, 2014, 11, 4339-4349.	4.6	31
33	Examining the limits of time reweighting and Kramersâ€™ rate theory to obtain correct kinetics from accelerated molecular dynamics. Journal of Chemical Physics, 2010, 132, 224101.	3.0	30
34	Improved Statistical Sampling and Accuracy with Accelerated Molecular Dynamics on Rotatable Torsions. Journal of Chemical Theory and Computation, 2012, 8, 4004-4012.	5.3	30
35	Identification of an l-Phenylalanine Binding Site Enhancing the Cooperative Responses of the Calcium-sensing Receptor to Calcium. Journal of Biological Chemistry, 2014, 289, 5296-5309.	3.4	30
36	The Cluster of Hydrophobic Residues Controls the Entrance to the Active Site of Choline Oxidase. Biochemistry, 2009, 48, 9599-9605.	2.5	29

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37	Extracting Realistic Kinetics of Rare Activated Processes from Accelerated Molecular Dynamics Using Kramersâ€™ Theory. Journal of Chemical Theory and Computation, 2011, 7, 575-581.	5.3	29
38	Molecular Cycloencapsulation Augments Solubility and Improves Therapeutic Index of Brominated Noscapine in Prostate Cancer Cells. Molecular Pharmaceutics, 2012, 9, 1470-1480.	4.6	29
39	Atomistic basis for the on-off signaling mechanism in SAM-II riboswitch. Nucleic Acids Research, 2010, 38, 1392-1400.	14.5	26
40	Enhanced molecular dynamics sampling of drug target conformations. Biopolymers, 2016, 105, 35-42.	2.4	26
41	Waterâ€™s Contribution to the Energetic Roughness from Peptide Dynamics. Journal of Chemical Theory and Computation, 2010, 6, 2591-2597.	5.3	25
42	Conformational Selection in the Recognition of Phosphorylated Substrates by the Catalytic Domain of Human Pin1. Biochemistry, 2011, 50, 9605-9615.	2.5	24
43	Enzyme-Mediated Conversion of Flavin Adenine Dinucleotide (FAD) to 8-Formyl FAD in Formate Oxidase Results in a Modified Cofactor with Enhanced Catalytic Properties. Biochemistry, 2017, 56, 3800-3807.	2.5	23
44	Atomic-level insights into metabolite recognition and specificity of the SAM-II riboswitch. Rna, 2012, 18, 300-307.	3.5	22
45	Conformation-Directed Catalysis and Coupled Enzymeâ€“Substrate Dynamics in Pin1 Phosphorylation-Dependent Cisâ€“Trans Isomerase. Journal of Physical Chemistry B, 2013, 117, 11509-11517.	2.6	22
46	Extracellular Calcium Modulates Actions of Orthosteric and Allosteric Ligands on Metabotropic Glutamate Receptor 1Î±. Journal of Biological Chemistry, 2014, 289, 1649-1661.	3.4	22
47	Achieving Rigorous Accelerated Conformational Sampling in Explicit Solvent. Journal of Physical Chemistry Letters, 2014, 5, 1217-1224.	4.6	22
48	Cysteine-Mediated Dynamic Hydrogen-Bonding Network in the Active Site of Pin1. Biochemistry, 2014, 53, 3839-3850.	2.5	22
49	Establishing a Framework of Using Residueâ€“Residue Interactions in Protein Difference Network Analysis. Journal of Chemical Information and Modeling, 2019, 59, 3222-3228.	5.4	21
50	Insights on the Mechanism of Amine Oxidation Catalyzed by <scp>d</scp>-Arginine Dehydrogenase Through pH and Kinetic Isotope Effects. Journal of the American Chemical Society, 2011, 133, 18957-18965.	13.7	20
51	Synthesis and effect of heterocycle modification on the spectroscopic properties of a series of unsymmetrical trimethine cyanine dyes. Dyes and Pigments, 2014, 105, 238-249.	3.7	20
52	Coupled Dynamics and Entropic Contribution to the Allosteric Mechanism of Pin1. Journal of Physical Chemistry B, 2016, 120, 8405-8415.	2.6	20
53	Novel third-generation water-soluble noscapine analogs as superior microtubule-interfering agents with enhanced antiproliferative activity. Biochemical Pharmacology, 2014, 92, 192-205.	4.4	19
54	Role of Ca2+ and L-Phe in Regulating Functional Cooperativity of Disease-Associated â€œToggleâ€• Calcium-Sensing Receptor Mutations. PLoS ONE, 2014, 9, e113622.	2.5	18

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55	Importance of Loop L1 Dynamics for Substrate Capture and Catalysis in Pseudomonas aeruginosa <scp>d</scp>-Arginine Dehydrogenase. Biochemistry, 2017, 56, 2477-2487.	2.5	18
56	Unraveling Allosteric Mechanisms of Enzymatic Catalysis with an Evolutionary Analysis of Residueâ€“Residue Contact Dynamical Changes. ACS Catalysis, 2018, 8, 2375-2384.	11.2	18
57	An Iron Reservoir to the Catalytic Metal. Journal of Biological Chemistry, 2015, 290, 15621-15634.	3.4	17
58	Detecting Functional Dynamics in Proteins with Comparative Perturbed-Ensembles Analysis. Accounts of Chemical Research, 2019, 52, 3455-3464.	15.6	17
59	Mapping the tropomyosin isoform 5 binding site on human erythrocyte tropomodulin: Further insights into E-Tmod/TM5 interaction. Archives of Biochemistry and Biophysics, 2005, 444, 130-138.	3.0	16
60	Cyclophilin A Inhibition: Targeting Transition-State-Bound Enzyme Conformations for Structure-Based Drug Design. Journal of Chemical Information and Modeling, 2013, 53, 403-410.	5.4	15
61	Accelerated entropy estimates with accelerated dynamics. Journal of Chemical Physics, 2007, 127, 154105.	3.0	14
62	Entropic and Surprisingly Small Intramolecular Polarization Effects in the Mechanism of Cyclophilin A. Journal of Physical Chemistry B, 2012, 116, 10771-10778.	2.6	14
63	Residueâ€“Residue Contact Changes during Functional Processes Define Allosteric Communication Pathways. Journal of Chemical Theory and Computation, 2022, 18, 1173-1187.	5.3	14
64	Decoding Allosteric Communication Pathways in Cyclophilin A with a Comparative Analysis of Perturbed Conformational Ensembles. Journal of Physical Chemistry B, 2018, 122, 6528-6535.	2.6	13
65	Fe(II)/Fe(III) Redox Process Can Significantly Modulate the Conformational Dynamics and Electrostatics of Pirin in NF-ÎºB Regulation. ACS Omega, 2016, 1, 837-842.	3.5	12
66	Solvent-Slaved Motions in the Hydride Tunneling Reaction Catalyzed by Human Glycolate Oxidase. ACS Catalysis, 2016, 6, 2113-2120.	11.2	12
67	Substrate Sequence Determines Catalytic Activities, Domain-Binding Preferences, and Allosteric Mechanisms in Pin1. Journal of Physical Chemistry B, 2018, 122, 6521-6527.	2.6	12
68	Donor acceptor fluorophores: synthesis, optical properties, TD-DFT and cytotoxicity studies. Organic and Biomolecular Chemistry, 2021, 19, 1835-1846.	2.8	12
69	Computational perspective and evaluation of plausible catalytic mechanisms of peptidyl-prolyl cisâ€“trans isomerases. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 1994-2004.	2.4	11
70	Design, synthesis and biological evaluation of di-substituted noscapine analogs as potent and microtubule-targeted anticancer agents. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 2133-2140.	2.2	11
71	Redox-Specific Allosteric Modulation of the Conformational Dynamics of ÎºB DNA by Pirin in the NF-ÎºB Supramolecular Complex. Biochemistry, 2017, 56, 5002-5010.	2.5	11
72	Role of F357 as an Oxygen Gate in the Oxidative Half-Reaction of Choline Oxidase. Biochemistry, 2016, 55, 1473-1484.	2.5	10

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73	Structural mechanism of cooperative regulation of calcium-sensing receptor-mediated cellular signaling. Current Opinion in Physiology, 2020, 17, 269-277.	1.8	10
74	Tuning Protein Dynamics to Sense Rapid Endoplasmicâ€Reticulum Calcium Dynamics. Angewandte Chemie - International Edition, 2021, 60, 23289-23298.	13.8	10
75	Dynamical role of phosphorylation on serine/threonine-proline Pin1 substrates from constant force molecular dynamics simulations. Journal of Chemical Physics, 2015, 142, 075102.	3.0	9
76	Synergistic mutations in soluble guanylyl cyclase (sGC) reveal a key role for interfacial regions in the sGC activation mechanism. Journal of Biological Chemistry, 2019, 294, 18451-18464.	3.4	8
77	N-Glycosylation and Gaucher Disease Mutation Allosterically Alter Active-Site Dynamics of Acid-Î²-Glucosidase. ACS Catalysis, 2020, 10, 1810-1820.	11.2	8
78	p53 Is Potentially Regulated by Cyclophilin D in the Triple-Proline Loop of the DNA Binding Domain. Biochemistry, 2021, 60, 597-606.	2.5	8
79	The Dilemma of Conformational Dynamics in Enzyme Catalysis: Perspectives from Theory and Experiment. Advances in Experimental Medicine and Biology, 2014, 805, 221-243.	1.6	7
80	Second Generation G-Quadruplex Stabilizing Trimethine Cyanines. Bioconjugate Chemistry, 2019, 30, 2647-2663.	3.6	7
81	A Single-Point Mutation in <scp>d</scp>-Arginine Dehydrogenase Unlocks a Transient Conformational State Resulting in Altered Cofactor Reactivity. Biochemistry, 2021, 60, 711-724.	2.5	7
82	Intricacies of interactions, dynamics and solvent effects in enzyme catalysis: a computational perspective on cyclophilin A. Molecular Simulation, 2014, 40, 765-776.	2.0	6
83	Pushing the Limits of a Molecular Mechanics Force Field To Probe Weak CHÂ·Â·Â·Ï€ Interactions in Proteins. Journal of Chemical Theory and Computation, 2015, 11, 1854-1863.	5.3	5
84	Oscillatory Diffusion and Second-Order Cyclostationarity in Alanine Tripeptide from Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2016, 12, 372-382.	5.3	5
85	Combinatorial Coarse-Graining of Molecular Dynamics Simulations for Detecting Relationships between Local Configurations and Overall Conformations. Journal of Chemical Theory and Computation, 2018, 14, 6026-6034.	5.3	5
86	Subsets of adjacent nodes (SOAN): a fast method for computing suboptimal paths in protein dynamic networks. Molecular Physics, 2021, 119, .	1.7	5
87	From Distinct to Differential Conformational Dynamics to Map Allosteric Communication Pathways in Proteins. Journal of Physical Chemistry B, 2022, 126, 2612-2620.	2.6	5
88	Chapter 12 Accelerating Conformational Transitions in Biomolecular Simulations. Annual Reports in Computational Chemistry, 2006, 2, 221-232.	1.7	4
89	Conserved Hydration Sites in Pin1 Reveal a Distinctive Water Recognition Motif in Proteins. Journal of Chemical Information and Modeling, 2016, 56, 139-147.	5.4	4
90	Loss of intramolecular electrostatic interactions and limited conformational ensemble may promote self-association ofcis-tau peptide. Proteins: Structure, Function and Bioinformatics, 2015, 83, 436-444.	2.6	3

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91	Allosteric Fine-Tuning of the Binding Pocket Dynamics in the ITK SH2 Domain by a Distal Molecular Switch: An Atomistic Perspective. Journal of Physical Chemistry B, 2017, 121, 6131-6138.	2.6	3
92	Tuning Protein Dynamics to Sense Rapid Endoplasmicâ€Reticulum Calcium Dynamics. Angewandte Chemie, 2021, 133, 23477.	2.0	2
93	Editorial. Computational Biology and Chemistry, 2020, 89, 107373.	2.3	0