Yinglong Miao

List of Publications by Year in descending order

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102 papers	4,864 citations	117619 34 h-index	110368 64 g-index
117 all docs	117 docs citations	117 times ranked	4128 citing authors

#	Article	IF	Citations
1	Gaussian Accelerated Molecular Dynamics: Unconstrained Enhanced Sampling and Free Energy Calculation. Journal of Chemical Theory and Computation, 2015, 11, 3584-3595.	5.3	544
2	Improved Reweighting of Accelerated Molecular Dynamics Simulations for Free Energy Calculation. Journal of Chemical Theory and Computation, 2014, 10, 2677-2689.	5.3	344
3	Ensemble Docking in Drug Discovery. Biophysical Journal, 2018, 114, 2271-2278.	0.5	318
4	Activation and dynamic network of the M2 muscarinic receptor. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 10982-10987.	7.1	210
5	Unconstrained enhanced sampling for free energy calculations of biomolecules: a review. Molecular Simulation, 2016, 42, 1046-1055.	2.0	139
6	Accelerated molecular dynamics simulations of protein folding. Journal of Computational Chemistry, 2015, 36, 1536-1549.	3.3	134
7	CRISPR-Cas9 conformational activation as elucidated from enhanced molecular simulations. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 7260-7265.	7.1	133
8	Graded activation and free energy landscapes of a muscarinic G-proteinâ€“coupled receptor. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 12162-12167.	7.1	132
9	Accelerated molecular dynamics simulations of ligand binding to a muscarinic G-protein-coupled receptor. Quarterly Reviews of Biophysics, 2015, 48, 479-487.	5.7	127
10	Gaussian accelerated molecular dynamics: Principles and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1521.	14.6	127
11	Gaussian Accelerated Molecular Dynamics in NAMD. Journal of Chemical Theory and Computation, 2017, 13, 9-19.	5.3	117
12	Mechanism of the G-protein mimetic nanobody binding to a muscarinic G-protein-coupled receptor. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 3036-3041.	7.1	111
13	Gaussian Accelerated Molecular Dynamics: Theory, Implementation, and Applications. Annual Reports in Computational Chemistry, 2017, 13, 231-278.	1.7	107
14	Ligand Gaussian Accelerated Molecular Dynamics (LiGaMD): Characterization of Ligand Binding Thermodynamics and Kinetics. Journal of Chemical Theory and Computation, 2020, 16, 5526-5547.	5.3	105
15	Striking Plasticity of CRISPR-Cas9 and Key Role of Non-target DNA, as Revealed by Molecular Simulations. ACS Central Science, 2016, 2, 756-763.	11.3	103
16	Deciphering Off-Target Effects in CRISPR-Cas9 through Accelerated Molecular Dynamics. ACS Central Science, 2019, 5, 651-662.	11.3	99
17	Population Based Reweighting of Scaled Molecular Dynamics. Journal of Physical Chemistry B, 2013, 117, 12759-12768.	2.6	94
18	Positive allosteric mechanisms of adenosine A1 receptor-mediated analgesia. Nature, 2021, 597, 571-576.	27.8	84

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19	Accelerated structure-based design of chemically diverse allosteric modulators of a muscarinic G protein-coupled receptor. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E5675-84.	7.1	82
20	G-protein coupled receptors: advances in simulation and drug discovery. Current Opinion in Structural Biology, 2016, 41, 83-89.	5.7	80
21	Mechanistic Insights into Specific G Protein Interactions with Adenosine Receptors. Journal of Physical Chemistry B, 2019, 123, 6462-6473.	2.6	80
22	Allosteric Effects of Sodium Ion Binding on Activation of the M3 Muscarinic G-Protein-Coupled Receptor. Biophysical Journal, 2015, 108, 1796-1806.	0.5	79
23	Peptide Gaussian accelerated molecular dynamics (Pep-GaMD): Enhanced sampling and free energy and kinetics calculations of peptide binding. Journal of Chemical Physics, 2020, 153, 154109.	3.0	77
24	Free energy landscape of G-protein coupled receptors, explored by accelerated molecular dynamics. Physical Chemistry Chemical Physics, 2014, 16, 6398.	2.8	74
25	Structural Basis for Binding of Allosteric Drug Leads in the Adenosine A1 Receptor. Scientific Reports, 2018, 8, 16836.	3.3	63
26	All-Atom Multiscale Simulation of Cowpea Chlorotic Mottle Virus Capsid Swelling. Journal of Physical Chemistry B, 2010, 114, 11181-11195.	2.6	60
27	Improved Modeling of Peptide-Protein Binding Through Global Docking and Accelerated Molecular Dynamics Simulations. Frontiers in Molecular Biosciences, 2019, 6, 112.	3.5	60
28	Multi-Conformer Ensemble Docking to Difficult Protein Targets. Journal of Physical Chemistry B, 2015, 119, 1026-1034.	2.6	59
29	Identification of SLAC1 anion channel residues required for CO ₂ /bicarbonate sensing and regulation of stomatal movements. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 11129-11137.	7.1	58
30	Ligand Binding Pathways and Conformational Transitions of the HIV Protease. Biochemistry, 2018, 57, 1533-1541.	2.5	52
31	Derivation of Mean-Square Displacements for Protein Dynamics from Elastic Incoherent Neutron Scattering. Journal of Physical Chemistry B, 2012, 116, 5028-5036.	2.6	48
32	Mapping of Allosteric Druggable Sites in Activationâ€Associated Conformers of the M2 Muscarinic Receptor. Chemical Biology and Drug Design, 2014, 83, 237-246.	3.2	43
33	Temperature-Dependent Dynamical Transitions of Different Classes of Amino Acid Residue in a Globular Protein. Journal of the American Chemical Society, 2012, 134, 19576-19579.	13.7	41
34	Acceleration of biomolecular kinetics in Gaussian accelerated molecular dynamics. Journal of Chemical Physics, 2018, 149, 072308.	3.0	41
35	Viral structural transitions: An all-atom multiscale theory. Journal of Chemical Physics, 2006, 125, 214901.	3.0	37
36	Gaussian accelerated molecular dynamics for elucidation of drug pathways. Expert Opinion on Drug Discovery, 2018, 13, 1055-1065.	5.0	37

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37	Mechanisms of Î³-Secretase Activation and Substrate Processing. ACS Central Science, 2020, 6, 969-983.	11.3	34
38	All-atom multiscaling and new ensembles for dynamical nanoparticles. Journal of Chemical Physics, 2006, 125, 044901.	3.0	32
39	Stochastic dynamics of bionanosystems: Multiscale analysis and specialized ensembles. Journal of Chemical Physics, 2008, 128, 234908.	3.0	32
40	Gâ€Proteinâ€Coupled Receptorâ€“Membrane Interactions Depend on the Receptor Activation State. Journal of Computational Chemistry, 2020, 41, 460-471.	3.3	32
41	Molecular dynamics/order parameter extrapolation for bionanosystem simulations. Journal of Computational Chemistry, 2009, 30, 423-437.	3.3	30
42	Replica Exchange Gaussian Accelerated Molecular Dynamics: Improved Enhanced Sampling and Free Energy Calculation. Journal of Chemical Theory and Computation, 2018, 14, 1853-1864.	5.3	29
43	Proteinâ€“Protein Interaction-Gaussian Accelerated Molecular Dynamics (PPI-GaMD): Characterization of Protein Binding Thermodynamics and Kinetics. Journal of Chemical Theory and Computation, 2022, 18, 1275-1285.	5.3	29
44	GLOW: A Workflow Integrating Gaussian-Accelerated Molecular Dynamics and Deep Learning for Free Energy Profiling. Journal of Chemical Theory and Computation, 2022, 18, 1423-1436.	5.3	29
45	Molecular dynamic study of MlaC protein in Gramâ€negative bacteria: conformational flexibility, solvent effect and proteinâ€phospholipid binding. Protein Science, 2016, 25, 1430-1437.	7.6	26
46	Mechanism of Tripeptide Trimming of Amyloid Î²-Peptide 49 by Î³-Secretase. Journal of the American Chemical Society, 2022, 144, 6215-6226.	13.7	26
47	Coupled Flexibility Change in Cytochrome P450cam Substrate Binding Determined by Neutron Scattering, NMR, and Molecular Dynamics Simulation. Biophysical Journal, 2012, 103, 2167-2176.	0.5	25
48	Mapping the allosteric sites of the A_{2A} adenosine receptor. Chemical Biology and Drug Design, 2018, 91, 5-16.	3.2	25
49	Self-assembly of nanocomponents into composite structures: Derivation and simulation of Langevin equations. Journal of Chemical Physics, 2009, 130, 194115.	3.0	24
50	Active-Site Hydration and Water Diffusion in Cytochrome P450cam: AÂHighly Dynamic Process. Biophysical Journal, 2011, 101, 1493-1503.	0.5	23
51	A Computational Modeling Approach Predicts Interaction of the Antifungal Protein AFP from Aspergillus giganteus with Fungal Membranes via Its Î³-Core Motif. MSphere, 2018, 3, .	2.9	22
52	Viral structural transition mechanisms revealed by multiscale molecular dynamics/order parameter extrapolation simulation. Biopolymers, 2010, 93, 61-73.	2.4	20
53	Reactive Center Loop Insertion in Î±-1-Antitrypsin Captured by Accelerated Molecular Dynamics Simulation. Biochemistry, 2017, 56, 634-646.	2.5	20
54	Recognition of single-stranded nucleic acids by small-molecule splicing modulators. Nucleic Acids Research, 2021, 49, 7870-7883.	14.5	18

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55	Identification and Validation of an Aspergillus nidulans Secondary Metabolite Derivative as an Inhibitor of the Musashi-RNA Interaction. Cancers, 2020, 12, 2221.	3.7	17
56	Pathway and mechanism of drug binding to chemokine receptors revealed by accelerated molecular simulations. Future Medicinal Chemistry, 2020, 12, 1213-1225.	2.3	17
57	Mechanism of RNA recognition by a Musashi RNA-binding protein. Current Research in Structural Biology, 2022, 4, 10-20.	2.2	17
58	Space Warping Order Parameters and Symmetry: Application to Multiscale Simulation of Macromolecular Assemblies. Journal of Physical Chemistry B, 2012, 116, 8423-8434.	2.6	16
59	Quasielastic neutron scattering in biology: Theory and applications. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 3638-3650.	2.4	15
60	Structure of the Human Respiratory Syncytial Virus M2-1 Protein in Complex with a Short Positive-Sense Gene-End RNA. Structure, 2020, 28, 979-990.e4.	3.3	15
61	<scp>A</scp>ctivation mechanisms of the first sphingosineâ€1â€phosphate receptor. Protein Science, 2017, 26, 1150-1160.	7.6	13
62	Retrospective ensemble docking of allosteric modulators in an adenosine G-protein-coupled receptor. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129615.	2.4	13
63	Structure and mechanism of the Î³-secretase intramembrane protease complex. Current Opinion in Structural Biology, 2022, 74, 102373.	5.7	13
64	Structures of Î²1-adrenergic receptor in complex with Gs and ligands of different efficacies. Nature Communications, 2022, 13, .	12.8	13
65	Mechanism of Ligand Recognition by Human ACE2 Receptor. Journal of Physical Chemistry Letters, 2021, 12, 4814-4822.	4.6	12
66	Investigation of the conformational dynamics of the apo A_{2A} adenosine receptor. Protein Science, 2015, 24, 1004-1012.	7.6	11
67	Recent advances in computational studies of GPCR-G protein interactions. Advances in Protein Chemistry and Structural Biology, 2019, 116, 397-419.	2.3	11
68	Ligand Binding in the Extracellular Vestibule of the Neurotransmitter Transporter Homologue LeuT. ACS Chemical Neuroscience, 2017, 8, 619-628.	3.5	10
69	Agonist Binding and G Protein Coupling in Histamine H2 Receptor: A Molecular Dynamics Study. International Journal of Molecular Sciences, 2020, 21, 6693.	4.1	10
70	General trends of dihedral conformational transitions in a globular protein. Proteins: Structure, Function and Bioinformatics, 2016, 84, 501-514.	2.6	8
71	Pathways and Mechanism of Caffeine Binding to Human Adenosine A2A Receptor. Frontiers in Molecular Biosciences, 2021, 8, 673170.	3.5	8
72	Zaccai neutron resilience and site-specific hydration dynamics in a globular protein. European Physical Journal E, 2013, 36, 72.	1.6	7

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73	An Efficient Gaussian-Accelerated Molecular Dynamics (GaMD) Multilevel Enhanced Sampling Strategy: Application to Polarizable Force Fields Simulations of Large Biological Systems. Journal of Chemical Theory and Computation, 2022, 18, 968-977.	5.3	6
74	Molecular Simulations and Drug Discovery of Adenosine Receptors. Molecules, 2022, 27, 2054.	3.8	6
75	Docking simulation and antibiotic discovery targeting the MlaC protein in Gramâ€negative bacteria. Chemical Biology and Drug Design, 2019, 93, 647-652.	3.2	5
76	Binding Analysis Using Accelerated Molecular Dynamics Simulations and Future Perspectives. Advances and Applications in Bioinformatics and Chemistry, 2022, Volume 15, 1-19.	2.6	5
77	Specific Engineered G Protein Coupling to Histamine Receptors Revealed from Cellular Assay Experiments and Accelerated Molecular Dynamics Simulations. International Journal of Molecular Sciences, 2021, 22, 10047.	4.1	4
78	Unique features of different classes of <scp>Gâ€proteinâ€coupled</scp> receptors revealed from sequence coevolutionary and structural analysis. Proteins: Structure, Function and Bioinformatics, 2022, 90, 601-614.	2.6	4
79	Mechanism of tethered agonist-mediated signaling by polycystin-1. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2113786119.	7.1	4
80	Computer-aided GPCR drug discovery. , 2020, , 283-293.		3
81	Molecular Mechanism of Off-Target Effects in CRISPR-Cas9. Biophysical Journal, 2019, 116, 319a.	0.5	2
82	Ligand Gaussian Accelerated Molecular Dynamics (LiGaMD) for Characterization of Ligand Binding Thermodynamics and Kinetics. Biophysical Journal, 2021, 120, 97a.	0.5	2
83	Efficient purification and assembly of ribonucleoprotein complex for interaction analysis by MST assay coupled with GaMD simulations. STAR Protocols, 2021, 2, 100315.	1.2	2
84	Mechanism of Peptide Agonist Binding in CXCR4 Chemokine Receptor. Frontiers in Molecular Biosciences, 2022, 9, 821055.	3.5	2
85	Enhanced Conformational Sampling of M2 Muscarinic Acetylcholine Receptor for Designing Selective Allosteric Drugs. Biophysical Journal, 2013, 104, 26a.	0.5	1
86	Hybrid finite element and Brownian dynamics method for charged particles. Journal of Chemical Physics, 2016, 144, 164107.	3.0	1
87	Accelerated Molecular Dynamics Simulations of Protein Folding. Journal of Computational Chemistry, 2016, 37, .	3.3	1
88	Enhanced Sampling of Peptide Binding to Proteins through Gaussian Accelerated Molecular Dynamics Simulations. Biophysical Journal, 2020, 118, 139a.	0.5	1
89	Mechanism and Pathways of Inhibitor Binding to the Human ACE2 Receptor for SARS-CoV1/2. Biophysical Journal, 2021, 120, 204a.	0.5	1
90	Dynamics Investigation of the Cytochrome P450cam Active Site Mutant Thr252ALA. Biophysical Journal, 2011, 100, 222a.	0.5	0

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91	Temperature Dependent Dynamics of Cytochrome P450cam from Elastic Incoherent Neutron Scattering. Biophysical Journal, 2012, 102, 382a.	0.5	0
92	Activation of the M2 Muscarinic Receptor and Computer-Aided Design of Receptor-Selective Allosteric Drugs. Biophysical Journal, 2014, 106, 101a.	0.5	0
93	Activation and Drug Design of a Muscarinic G-Protein Coupled Receptor. Biophysical Journal, 2015, 108, 95a.	0.5	0
94	Activation of a Muscarinic G-Protein Coupled Receptor and Structure-Based Design of Allosteric Modulators. Biophysical Journal, 2016, 110, 426a-427a.	0.5	0
95	CRISPR-Cas9: Computational Insights Toward Improved Genome Editing. Biophysical Journal, 2017, 112, 72a.	0.5	0
96	Enhanced Simulations and Drug Discovery of a Muscarinic G-Protein-Coupled Receptor. Biophysical Journal, 2017, 112, 328a-329a.	0.5	0
97	A PAM-Induced Signalling Activates the Communication between HNH and RUVC in CRISPR-Cas9. Biophysical Journal, 2018, 114, 250a.	0.5	0
98	Gaussian-Accelerated Molecular Dynamics Modeling Leads to Identification of SLAC1 Anion Channel Residues for CO2 Signaling in Arabidopsis Guard Cell. Biophysical Journal, 2018, 114, 302a.	0.5	0
99	Mechanism of Specific G Protein Coupling to Adenosine Receptors. Biophysical Journal, 2019, 116, 176a.	0.5	0
100	Peptide Gaussian Accelerated Molecular Dynamics (Pep-GaMD) Enhanced Sampling and Free Energy and Kinetics Calculations of Peptide Binding. Biophysical Journal, 2021, 120, 97a.	0.5	0
101	Mechanisms of Tethered-Ligand Mediated Polycystin-1 GPCR Signaling. Biophysical Journal, 2021, 120, 304a.	0.5	0
102	Structure of the human respiratory syncytial virus M2-1 protein in complex with a short positive-sense gene-end RNA. Acta Crystallographica Section A: Foundations and Advances, 2020, 76, a117-a117.	0.1	0